# Details of 2021 Designated Research Areas

## ① Mathematics / Computer science

### ■ Mathematics for scientific computing and machine learning

*(Designated in 2012, revised in 2019, 2021)*

(Research trends) Mathematics has been widely applied to problems which arise in various areas such as science, engineering, and industry. In recent years, the mechanism of machine learning has risen to a significant area of interest. A majority consists in the development of mathematical theories, modeling of situations, and visualization of phenomena. Recent advances in deep learning are expected to upend some of the limitations of existing mathematical frameworks in dealing with various ill-posed problems, e.g., modeling complicated datasets, image reconstruction with insufficient data, and solving high-dimensional partial differential equations.

(Necessity for IBS) Existing numerical approaches are computationally expensive, hence, their practical use has been limited due to the curse of dimensionality. Also, there is a lack of numerical methods to approximate general solutions for various problem settings, such as different boundary conditions, initial conditions and physical setups. Therefore, there is a significant need for developing numerical methodology to solve partial differential equations in various setting with reasonable computational cost.

Although deep learning has accomplished great successes in various areas including science and medicine, there is a tremendous lack of a rigorous mathematical foundation that would allow us to understand why deep learning methods perform that well. Hence, there is a great need to develop mathematical theories to ascertain not only their reliabilities but also interpretability from the human perspective.

Most research paradigms in deep learning are becoming interdisciplinary in nature, involving mathematics, data science, computational engineering, and medicine. Collaborative research among mathematics and other fields is necessary to achieve a balance among theoretical ground, intuition, and applications.

(Key research contents) The research topics of the Center are as follows.

[Mathematics]

1) Numerical analysis

· Numerical schemes for differential equations

· Computational complexity

2) Discrete mathematics

· Graph theory for data analysis

3) Probability theory

· Bayesian data analysis
· Statistical learning
· Causality

4) Optimal transport

· Domain adaptation

5) Mathematical foundation for deep learning

· Universal approximation
· Optimization

[Applications]

1) Image enhancement

· Denoising
· Deblurring
· Super-resolution

2) Image generation

· Development of new architectures for generative models
· Evaluation metric for generative models

3) Anomaly detection

· Visual inspection for industrial data

4) Representation learning

· Contrastive learning

5) Recommendation system

· Graph neural networks for recommendation

6) Interdisciplinary researches in the various fields

· Numerical simulation in computer science, engineering, biology or genomics
· Image analysis in physics, chemistry, biology or medical sciences

7) Other emerging field

## ■ Arithmetic and algebraic structure *(Designated in 2012, revised in 2019)*

This area allows the development of solutions to problems in algebra and arithmetic geometry, while, at the same time, applying such solutions to various problems in information science, e.g. cryptology through full computer implementations.

- Arithmetic: Study of algebraic integers and integral solutions of equations with integral coefficients
- Modular form: Arithmetic and analytic properties of modular forms
- Moduli: Study of variation in algebraic structures
- Representation: Unifying study of linear transformations in various areas of mathematics
- Cryptography: Mathematical theories underpinning the secure exchange of information
- Coding: Mathematical theory for compression and error correction in information exchange
- Including but not limited to the above areas of study

## ■ Randomness *(Designated in 2012, revised in 2019)*

The notion of randomness is gradually playing more important roles in many problems of mathematical nature, and work in this area has far-reaching consequences across many other disciplines. It is a central notion in understanding complex systems, like social networks; and applied probability and statistics have become essential tools for the study of many questions connected to biology and industrial problems.

- Randomness: Random properties of complex systems, Probability and mathematical statistics
- Random Matrix: Study of matrix valued random variables
- Random Graph: Interaction between graph theory and probability
- Including but not limited to the above areas of study

## ■ Nonlinearity *(Designated in 2012, revised in 2019)*

Nonlinear phenomena are ubiquitous in nature. A large variety of fundamental phenomena occurring in science and engineering can be formulated in terms of nonlinear partial differential equations (PDEs). They include, among others, Navier-Stokes equations in fluid mechanics, elastic equations in solid mechanics, Einstein equations in general relativity, Yang-Mills equations in gauge theory and nonlinear equations describing optimal transport theory. Unlike linear equations, there are not many general theories applicable to all these equations simultaneously, and many fundamental mathematical questions, such as global existence in time, uniqueness, and stability of solutions and their implications, are still open. However, each of these fundamental PDEs carries its own hidden characteristics tied to its inherent nature, which help mathematicians solve the problems. Some of the universal characteristics are action principle (calculus of variation), Hamiltonian structure (integrable system), solitons, the formation of singularities (such as shock formation or black-hole formation), etc.

Recently, there have been great advances in our understanding of these nonlinear PDEs and their unexpected applications to the study of geometry and topology, such as the construction of exotic differentiable structures in space-time and Perelman's solution to Poincaré conjecture in topology. Recent advances in simulation also help our understanding of complex nonlinear phenomena, such as turbulence. Currently, nonlinear phenomena also play a primary role in addressing various nonlinear inverse problems in industry.

· Fluid/solid mechanics and conservation laws

· Kinetic equation and Hamilton-Jacobi equation

· Geometric partial differential equations

· Optimal transport

· Nonlinear inverse problems

· Mathematical modeling in nonlinear science and engineering

· Including but not limited to the above areas of study

■ **Dynamics** *(Designated in 2012, revised in 2019)*

The study of dynamics in mathematics deals with the understanding of the fundamental mechanisms of dynamical systems, and finds applications in mathematics, physics, as well as other scientific and engineering fields. The theory of dynamical systems is a fundamental part of chaos theory, logistic map dynamics, self-assembly and self-organization processes, etc. Besides its importance in mathematics and traditional applications, the area has recently witnessed spectacular applications to number theory, in helping to solve longstanding open problems, and started to have an impact in other fields.

· Discrete dynamical systems: Dynamical properties of iterations of transformations

· Stochastics and ergodicity: Stochastic and ergodic phenomena in various areas of mathematical sciences

· Bifurcation and chaos: Phase transition and statistical phenomena

· Computational dynamics and applications

· Including but not limited to the above areas of study

■ **Data Science** *(Designated in 2017, revised in 2019, 2021)*

(Research trends) One of the most crucial factors that enable automated systems via artificial intelligence (AI) is the emergence and powerful processing of high-dimensional Big Data in a variety of fields. On the other hand, statistical machine learning and deep learning is capable of effectively extracting features from high-dimensional data at the largest scale, resulting in recent breakthroughs in the implementation of AI-aided systems. Thus, it is strongly expected that data science methodologies, including statistical data processing, feature representation via deep learning, and parallel utilization of GPUs for large-scale data, will greatly facilitate the solution to plenty of challenging problems that remain open across diverse research areas.

As the first step, the data science group was launched in 2019 and has been working since then. In fact the data science group now covers only a small portion of this interdiscilinary area, such as the applcation of AI theory including data mining to various fields. Thus, it is necessary to nurture resaerch groups to develop the fundamental theory of data science and the emerging methodologies.

(Necessity for IBS) Interdisciplinary research on data science unifying statistics, data analysis and the related methods has still been lacking. To take an initiative in such direction, it would be necessary to establish a multidisciplinary Research Center on data science, which employs theories and techniques from a variety of fields, like mathematics, information science and computer science, and includes machine learning, data mining, databases, and visualizations. Such Center will be beneficial to the other IBS Research Centers for life science, medicine, physics, and chemistry, to boost their innovative scientific discoveries and develop state-of-the-art data science techniques.

(Key research contents) The research topics of the Data Science Center include 1) Fundamental theories for data science such as statistical processing and high-dimensional statistics; 2) Design of representation learning algorithms based on generative models so as to effectively conduct many supervised learning tasks with insufficient labeled data; 3) Development of computational infrastructures along with parallel computing; and 4) Applications of data science to system biology, health and medical science, physics, chemistry, astronomy, etc.

## ② Physics

### 1) Theoretical physics

**■ Theoretical fundamental physics** *(Designated in 2012, revised in 2019, 2021)*

**• Particle & nuclear theory** *(Designated in 2012, revised in 2021)*

Particle physics is at the forefront of pioneering basic science research, and essential to the generation of new knowledge. The goal of theoretical nuclear physics is to explain the structures and reactions of nucleons and nuclei using a single consistent theory that can describe all matter from microscopic quarks to macroscopic nuclei and celestial objects.

- Understanding of accelerator's experimental results and new particle phenomenology
- The particle theory of dark matter
- Research on the breaking of supersymmetry
- Understanding of strong-interaction systems based on superstring and M-theory
- Theory of dense hadronic matter
- QCD-based computational studies of high-energy phenomenology and nuclear structure
- In-depth understanding of renormalization models for nuclear force and QCD-based effective field theories
- Including but not limited to the above areas of study

Now that the Center is launched, it is highly desirable for other centers be established to cover the whole areas of the Theoretical Fundamental Physics and to carry out cooperative and complementary research through the co-directorship.

**• String theory & gravitation / field theory** *(Designated in 2012)*

The goal of this area is to address, within a single framework, numerous physics questions, including the fundamental interactions of nature, the fundamental explanation of matters, the understanding of the quantum theory of gravity in unusual systems, such as black holes, and the birth of the Universe.

- String-theory phenomenology
- Holography
- Theory of the D-branes and the M-branes
- AdS(Anti de Sitter space)/CFT(Conformal Field Theory)
- Non-perturbative field theory
- Quantum black hole and information puzzle
- Quantum gravity, and the theory of gravity in the supergravity environment
- Including but not limited to the above areas of study

• **Astrophysics & cosmology** *(Designated in 2012)*

Research in astrophysics and cosmology aims to enable the formulation of the most fundamental laws of nature, as well as to explain the space-time structure of the universe, and to produce a new paradigm for the origin of the matters and the laws of nature.

- Black holes, neutron stars, supernovae, gamma ray bursts, and Lorentz invariance
- Dark energy and relationship, the origin of the extreme energy, the era of darkness and reionization, and theoretical models for the black-hole formation and the star formation
- Identifying dark energy, dark matter and the space-time structure of the dark universe
- Evolution of the accelerating universe including the birth of stars and galaxies.
- Theoretical models on early universe
- Study of gravitational waves in early universe and their effects on the cosmic background radiation
- Including but not limited to the above areas of study

• **Other emerging research areas** *(Designated in 2019)*

■ **Condensed-matter and complex systems theory** *(Designated in 2012, revised in 2021)*

• **Strongly correlated electron systems** *(Designated in 2012, revised in 2019)*

(Research trends) Our understanding of quantum materials became broadened and also rapidly complicated because these materials often show a combination of strong correlation and novel crystal structures. In order to understand these new quantum states of matter, besides the traditional methods (such as symmetry breakings, new orders and collective excitations), we need to understand new organizing principles of materials/systems with strong correlations.

It is obvious that the fabrication and control of new functional materials will be a core part of the technological leadership of the 21st century, therefore the research on strongly correlated electronic systems (SCES) is a top priority of the national science policy for all advanced countries.

(Necessity for IBS) The investigation of SCES is an essential part of new material research both for applications as well as fundamental studies. As the initial stage in this field, IBS should establish a theoretical research group in addition to the already existing experimental group, the Center for Correlated Electron Systems (CCES). The collaborative research with CCES, as well as with the Center for Theoretical Physics of Complex Systems (PCS), will boost the synergy for the understanding of SCES.

(Key research contents) The research topics of the SCES group will include:

1) Crystalline materials with strong correlation. One century after the discovery of quantum mechanics, the understanding of crystalline materials with strong correlation – usually consisting of transition elements, and rare earth elements – still remains a grand challenge of theoretical physics.

2) Unconventional superconductivity. Topologically trivial and non-trivial superconductivity is a powerful platform to investigate correlated and topological quantum matters. It has also a great potential for applications, such as room-temperature superconductors and quantum computers.

- **Computational materials physics** *(Designated in 2012, revised in 2019)*

(Research trends) With the increasing power of ultrafast computers and the development of efficient algorithms, the computational approach has become an efficient exploratory tool for searching new materials with targeted physical properties, such as topological materials, magnets, multi-ferroics, and superconductors.

(Necessity for IBS) In recent years, the computational materials research has grown in scale and collaborative nature requiring large computational resources and manpower. Advanced countries like the US, Europe, and Japan have already established many dedicated research centers/institutes for computational materials research.

(Key research contents)
1) Quantum theory of materials. Based on an atomic, quantum mechanical description, materials theory aims to understand and predict the novel functional properties of the materials, such as superconductivity and topological phases. It can also design and propose new functional materials with desired properties. Ultimately, it will develop a powerful and comprehensive theoretical tool for new quantum materials.

2) Computational materials modeling. The dramatic growth in the capability of computational resources now allows many thousands of computations to be performed independently and at the same time. First-principles calculations combined with machine learning algorithms can efficiently screen for novel and extreme materials, using existing databases of crystal structures, or their modifications, and computing their properties. This research aims to predict room temperature superconductors, materials under extreme conditions, non-crystalline material structures, two-dimensional materials, biomaterials, or other materials for different applications, like catalysis, solar cell, battery, and sensor research.

- **Theoretical study of quantum information and technology** *(Designated in 2019)*

(Research trends) Quantum computer/cryptography is the new technological frontier of the 21st century. To realize these new technologies, many scientific disciplines need to collaborate together: theoretical physics, low-temperature physics, AMO-physics, semiconductor physics, superconductors, computer engineering, mathematics, etc. Among others, theoretical physics provides fundamental principles, ideas, and a roadmap guiding the realization of quantum computer technology.
Moreover, the study of this field will also have a huge impact on quantum entanglement: our theoretical understanding and realistic manipulations.

(Necessity for IBS) Universities and national institutes as well as private sectors (Google, Microsoft, etc.) in the US, EU, and China are investing a huge sum of financial resources toward this direction. IBS is the ideal place for a theoretical Center for Quantum Information and Technology in Korea. This Center could carry on fundamental research on the theoretical aspects of quantum computer-related subjects and play a leadership role in orchestrating and utilizing the powerful, diverse expertise of domestic researchers.

(Key research contents)
1) Quantum information and entanglement. Quantum theory of many-body systems is still incomplete. Traditional theories, such as Hatree-Fock theory or perturbation theory, can deal with only a small class of quantum many-body states. To study the large unexplored quantum many-body states, the study of quantum information and entanglement is a new paradigm of theoretical approach to the quantum many-body system.

2) Quantum technology. Operations with qubits, quantum gates, quantum error corrections, etc. are building blocks for quantum computers and quantum simulators. A general principle of these Q-logic units should be developed and specific platforms such as cold atoms, Rydberg atoms, Josephson junctions, Majorana qubits, etc. should be studied.

- **Statistical physics** *(Designated in 2012, revised in 2021)*

(Research trends) Diverse phenomena emerging from many-body systems in far from equilibrium state still remain as central issues in statistical physics. The thermodynamic second law is reinterpreted from the perspective of so-called fluctuation theorems. The stochastic thermodynamics is newly setup and the concept of entropy production is widely applied to real systems in biophysics and information systems. This field expands rapidly and is even further progressed with the observation of thermodynamic uncertainty relation. Recently, stochastic dynamics is not limited to the Brownian case, but expanded to active particles with non-Gaussian noise. This active matter physics attracts considerable attention to biophysics community, because of the experimental feasibility. Various topics in complex systems are still interesting as an interdisciplinary subject. Complex network science is extended to for higher-order interacting systems in which interactions are among more than two individuals. Topological phase transitions in complex networks are also interesting in network science community, in which algebraic homology becomes one of the main tools. Phase transitions in complex systems and quantum systems are reconsidered using the machine learning algorithm.

(Necessity for IBS) The diverse subjects of statistical physics are investigated using diverse approaches; however, they need to be unified into a single framework. Accordingly, the research ground such as the IBS will be helpful for associated people to get together and share their perspectives with others.

(Key research contents) The research topics of the group for non-equilibrium statistical physics and complex systems will include:

1) Stochastic thermodynamics

2) Complex networks with higher order interactions

3) Dynamics in active matter systems

4) Understanding of diverse phase transitions arising in classical or closed and open quantum systems using the machine learning and artificial intelligent approaches.

- **Biological physics** *(Designated in 2012, revised in 2021)*

(Research trends) Biological physics has been seeking to answer the ultimate question of the materialistic and systemic basis for controlling and maintaining the living system. The inherent complexity involved with vastly different scales in time and length and the prevailing heterogeneity at every level of organization, from molecule to population, has made theoretical investigations heavily rely on molecular simulations or empirical model studies. However, recent advances in imaging techniques, complex systems theory and information technology brought new insights and perspectives to the fundamental problems of biophysics. Additionally, it led to surging demand in applied research in medicine and clinical biology. As a result, data science and machine intelligence components are gaining importance in theoretical biophysics, renewing interest in even more practical problems ranging from cancer to cell-based biochemical engineering to public health interventions in epidemics.

(Necessity for IBS) In light of imminent issues of contemporary life sciences, theoretical biophysics has traditionally focused on fundamental issues on a molecular or ecological scale. Quantitative understanding of intermediate-scale problems is largely lacking. Even on a molecular or cellular scale, the overwhelming complexity inherent in cancer heterogeneity, clinical genome editing, and working principle of the human brain has been holding back progress. But novel approaches, emerging from machine intelligence and stochastic thermodynamics, provides a promising breakthrough. Experimental verification is the ultimate must, but theoretical biophysics is arguably the investment of the highest benefit-cost ratios. As a primer, IBS should establish a theoretical research group that can first demonstrate synergy with the already existing experimental group in life sciences.

(Key research contents) The research topics of the group include:

1) Molecular/cellular biophysics: Understanding of 3D conformational dynamics of single biomolecules (e.g., proteins coupled with the cellular environment) in the context of biological functions. This field pertains to the traditional way of tackling the problems in biology. Yet, it requires even more aggressive effort that utilizes recent advances in the machine learning approach (e.g., AlphaFold). In addition, it can also include the discovery of new drug targets and rational drug design by using computational techniques as a subfield.

2) Statistical biophysics: Due to the overwhelming complexity in the underlying biological networks, the system-level understanding, let alone causal linking between molecular events and diseases, remains a grand challenge in biology. Participation by physicists and network scientists together will help to tackle the problems associated with genome-wide regulation. Systems biology and neuroscience, led by a leader (leaders) with a theoretical physics background, can be conceived as a part of this subfield. Our theoretical insight into biological phenomena gained from nonequilibrium statistical physics, network/data

science, and soft matter physics can be a core part of the leadership of biological physics in the coming decade.

3) Optimal design of biological systems: Living matter in action, at the smallest length scale epitomized by biological motors, operates out of equilibrium. Along with the microscopic underpinnings underlying the functions of individual motors, a new effort is burgeoning to quantify the flow of energy, information, and material balance in biological systems and address how it contributes to the cellular organizations.

• **Interdisciplinary studies** *(Designated in 2012)*

· The goal of this area is to invoke new developments in all fields of basic sciences, including physics, by extending the applications of physics and establishing a new paradigm.

· Theoretical and computational interdisciplinary studies: between physics and chemistry, between physics and biology, between physics and information sciences, between physics and economy, and between physics and sociology

· Including but not limited to the above areas of study

• **Other emerging research areas** *(Designated in 2019)*

## 2) Experimental physics

### ■ Multi-messenger science *(Designated in 2017, rev. 2021)*

(Research trends) Hundred years after Einstein's predictions, the recent direct detection of gravitational waves (GW) is not only a great, long-awaited success, which took more than 50 years of scientific efforts, but also a 'new window' to observe the Universe. Together with the rapidly developing electromagnetic (EM)-wave window and the precision-measurement neutrino window in astrophysics, GW open up a very challenging area of research: multi-messenger science. Worldwide competitions and ambitious projects in this new field have already started, and IBS should also be ready for this new 'Multi-messenger science-era' of astrophysics and cosmology. Present observatories for multi-messenger science LIGO/Virgo, and KAGRA for GW, Super-Kamiokande and IceCube for neutrinos, as well as multi-wavelength EM wave observatories including CMB observations and Pulsar Timing Array.

(Necessity for IBS) The Center for Multi-Messenger Science (of the Universe) aims to study various aspects of our Universe using multi-messenger observations, which provide ultimate clues in understanding many unsolved astrophysical and cosmological problems. The major components of multi-messenger observations are the new window recently opened by GW, and the precision-measurement windows of EM waves and cosmic neutrinos. A close interaction between this Center and other IBS Centers for theoretical physics and for dark matter search experiments is expected to generate a synergetic platform in understanding our Universe. The Center's GW and/or neutrino facilities are highly recommended to be built in the IBS's underground Yemi-lab or in the RAON site in order to create a physics research complex.

(Key research contents) The Center's research will cover the following areas:

1) Gravitational waves. Development of a new type of GW detector, preferably a novel compact design that allows to be built in the existing IBS sites such as the Yemi-lab underground hall or the RAON site. GW data analysis: test of general relativity and the equation of state of the neutron star. Theoretical/astrophysical studies of GW physics: GW sources, formation scenarios of compact binary objects, stochastic GW background and cosmology, etc.

2) EM waves. Precision observational astronomy is an essential part of multi-messenger observations. The wavelength of the observation spans from gamma rays to radio waves, including a rapid follow-up/coincident EM measurement of the GW and/or neutrino detections.

3) Neutrinos: Development of innovative design for a compact detector, preferably built in the existing IBS sites such as the Yemi-lab, to detect cosmic neutrino sources in cooperation with GW and/or EM wave observations, neutrino bursts from a supernova explosion in our Galaxy, as well as to determine the unknown properties of neutrinos beyond the scope of the Standard Model.

4) Other emerging new observational windows.

## ■ Experimental high energy physics *(Designated in 2019)*

(Research trends) Experimental particle physics has been the most influential field of physics for many decades. It also brought many revolutionary technologies and developed new industries. Medical technologies such as PET, cyber-knives, particle beam therapies, as well as computing applications, such as the WWW, grid computing, and neural networks (machine learning) have all originated from this field. The research area is often called high energy physics, and it also includes nuclear physics and astroparticle physics. The research relies on particle accelerators, detectors, and large computing facilities. The field is also associated with Big Science projects, as the number of collaborating physicists is often few hundreds to few thousands. The success story of CERN is well known to the public, and most of the top science students choose this field as their major. The field is mostly performed via large international collaborations which manage a huge research budget. Thus, a new trend in this field is sharing experimental facilities and research credits as well. This could be a particularly interesting feature for IBS, different from other science programs.

(Necessity for IBS) The Center for Experimental High Energy Physics aims to study particle physics as a member of international collaborations, which include Europe, the US, Japan, etc., and be recognized worldwide as the leading representative of Korea. The Center will focus on international collaborations, as opposed to all the other IBS Centers which perform in-land activities. Its top-edge researches will be carried out through accelerator-based experiments, either colliders or fixed targets. Ongoing experiments at the Large Hadron Collider (LHC) and some of the future collider programs, such as ILC, CEPC, CLIC, and FCC, can be imminent activities of the Center. B-Physics in KEK and at CERN can also be a good option for the Center. It will be composed of different research groups for activities in data analysis, Monte Carlo simulations, detector development and computing. The intensive research conducted by the Center will contribute to the fundamental understanding of nature and will also be able to provide technological breakthroughs in many application fields.

(Key research contents) The research areas of the Center are based on accelerators' experiments and include all features of the Standard Model and beyond the Standard Model, as well as the search for New Physics. The Center ideally consists of several subgroups, such as 1) Physics event generation (PYTHIA, MADGRAPH); 2) Detector MC simulation (GEANT4); 3) Data analysis; 4) Particle detector development (silicon vertex, tracking devices, EM and hadron calorimeters, muon detectors) and spin-off applications; 5) Large-scale Big Data software development and computation; and 6) Worldwide computing network construction (Tier1 and Tier2 level).

■ **Quantum information science** *(Designated in 2017, revised in 2021)*

(Research trends) Quantum technologies, including quantum computing, simulation, communication, and sensing, have the potential to revolutionize many fields of basic science and technology. This research area has originally developed from atomic, molecular and optical (AMO) physics, but its scope has been expanded to other fields of physics such as semiconductor and superconductor physics. It exploits a fundamentally new model of information processing, because it is based on the physical laws of quantum mechanics, instead of classical physics. It holds the promise of immense computing powers, beyond the capabilities of any classical computer, and guarantees absolutely secure communication. The worldwide interest and the importance of this area can be gauged by the recent significant increase of funding in the US, EU, UK, Canada, China, and Japan.

(Necessity for IBS) The Center for Quantum Information Science aims to extensively study physical principles of diverse quantum phenomena and to transfer the earned knowledge to future technologies. It is essential that the Center is composed of different research groups from diverse fields of physics including quantum optics, atomic/molecular physics, and semiconductor/superconductor physics. Both independent and interdependent research lines, as well as the close interaction between the groups, will guarantee complementary synergy effects to produce novel ideas and innovative technologies. The extensive but well-focused studies conducted in the Center will provide a strong foundation for understanding diverse quantum phenomena and concepts, and developing novel physical systems for quantum technologies.

(Key research contents) The research area of the Center will include 1) Fundamental quantum phenomena and technologies, such as quantum entanglement, qubit, Q-gate and quantum memory based on quantum optics, atomic & molecular physics (trapped ion/optical lattice clock), semiconductor physics (quantum dots, color center) and superconductor physics (Josephson, SQUID); 2) Diverse quantum systems to control quantum states through systems based on entangled single-photon sources, ion traps, SQUID, etc.; 3) Quantum cryptography, quantum computing and quantum network, including quantum repeater, quantum coding, quantum crypto/secure network, quantum information theory, quantum gate operation, and quantum simulators; 4) Many-body quantum phenomena, hybrid quantum systems and/or cold atoms/molecules; 5) Measurement techniques that are based on quantum entanglement and matter-wave interference.

## ■ Matter at extreme conditions *(Designated in 2019)*

(Research trends) One natural way to expand the horizon of our understanding of nature is to search for new materials and phases at extreme conditions. Indeed, most matter in the Universe, from the deep interior of planets to the core of stars, is at high temperature, pressure or magnetic field, in contrast to the matter of our ordinary experience. Among the many physics research areas, condensed matter is the one that is the most directly related to everyday life, leading to applications in modern IT and communications technologies. Condensed matter research grows into many directions: not only it analyses available materials, but also attempts to understand novel phenomena and design devices with desired functionalities. New materials or phases with exotic properties are in constant demand, as can be appreciated in the fields of unconventional superconductivity and topological materials. Recent discoveries of near-room-temperature superconductivity under high pressure are excellent examples. Ultra-high pressure not only allows us to have new materials and phases, but also mimics the condition inside the Earth. Thus, the study of matter at extreme conditions could naturally encompass geophysics, in particular mineral physics – the science of materials that compose the interior of the earth. Mineral physics would provide information that allows the interpretation of surface measurements of seismic waves, gravity anomalies, geomagnetic and electromagnetic fields, in terms of properties of the deep inner Earth.

(Necessity for IBS) Several physics areas have developed quickly in Korea after the establishment of IBS, whereas the study of matter at extreme conditions is still lagging behind. It is envisioned that this IBS center would act as a hub in bringing relevant scientists together and in raising the level of science to the global standard.

(Key research scopes) The following is a brief description of possible research areas in which the IBS Center for Matter at Extreme Conditions would excel: (1) Finding new materials and phases: Materials synthesis under high pressure, zero gravity and high magnetic fields; (2) Finding new novel phenomena: Various physical property measurements under high pressure, high electric/magnetic fields, ultra-low temperature or other extreme conditions; (3) Mineral physics in general; (4) Theory: Field theoretical as well as numerical approaches to the novel phenomena

## ■ Science of ultra-intense laser and matter interactions *(Designated in 2021)*

An ultra-high intensity laser can provide new opportunities for frontier science research, where extreme light-matter interactions are investigated. Nowadays a PW (peta-watt) laser is available, which is based on the chirped-pulse amplification method (a Nobel physics prize was awarded for this discovery in 2018), and this is an extremely important tool to study many physical phenomena in the universe from a microscopic level (atomic physics) to a macroscopic level (plasma physics and astrophysics). It offers new opportunities for fundamental physics research such as non-linear quantum electrodynamics (QED), laboratory astrophysics, high energy density (HED) physics, attosecond science, etc. This research also has many important applications, including compact ultrahigh intensity lasers, novel particle accelerators, extreme light sources for X-rays, gamma-rays, THz waves and EUV. Some (not all) important research subjects in science of ultraintense laser-matter interactions can be summarized as follows:

- Ultra-high intensity laser physics and technology: ultra-high intensity laser development, extreme field generation
- Strong field quantum electrodynamics (QED): nonlinear Compton scattering, Breit-Wheeler electron-positron pair production, vacuum birefringence, radiation reaction, QED cascades
- High energy density (HED) physics: relativistic pair (electron & positron) plasma, self-organization of HED plasma, dynamics of fully-evolved plasma turbulence
- Laboratory astrophysics: astrophysical QED phenomena, pulsar magnetosphere, cosmic ray acceleration, dwarf stars, solar interiors, relativistic shocks
- High energy particle generation: laser-driven electron and proton/ion acceleration with an extremely high acceleration gradient, generation of positrons and neutrons
- Extreme light source: novel X-ray, gamma-ray, THz wave, EUV sources
- High harmonic generation and attosecond science: high harmonic generation in gas/solid/plasma, generation/characterization of attosecond/zeptosecond pulses, ultrafast X-ray science

Current status of the research in Korea and necessity for IBS :

In 2016, a state-of-the-art 4 PW laser was developed and operated for the investigations of strong field physics research at Center for Relativistic Laser Science (CoReLS), Institute for Basic Science. Many technical obstacles were overcome with immense efforts and the laser system has been running with the highest peak power in stable conditions. In 2021, the record-breaking laser intensity of 1.1 $x10^{23}$ $W/cm^2$ was achieved. Such an ultrahigh power, ultrahigh intensity laser with good stability is very unique. Currently, the CoReLS PW laser, which is located on the campus of GIST (Gwangju Institute of Science and Technology), is the world's brightest and routinely operating laser. Compared to similar lasers in the US and Europe, it is at least a few years ahead of the leading PW laser facilities in peak power and intensity. Therefore, as the current director of CoReLS is retiring in August 2023, the establishment of a new IBS center pursuing innovative physics with this PW laser facility is much necessitated for boosting basic science in Korea. It can take advantage of the well-established laser and other facilities, including the 4 PW/1 PW beamlines, the 150 TW beamline, and the 20 mJ (1 kHz) Ti:sapphire laser, in exploring light-matter interactions in extreme spatio-temporal dimensions.

## ■ Quantum materials initiative: Emerging physical phenomena from nanoscale control *(Designated in 2021)*

(background) Applications for a new IBS center of nano-physics for the quantum material initiative are invited; the new center will be located at SKK Univ. as an extramural IBS center. This is a special and first attempt on the part of IBS because the new center will be allowed to take over all the facilities already installed by an out-going IBS center, the center for integrated nanostructure physics (CINAP). CINAP has operated various experimental equipments and facilities essential for cutting edge fundamental research in a wide range of categories such as (1) Clean room / Dry room, (2) Electric/thermal measurement, (3) Optics, (4) Structural analysis, and (5) Synthesis and fabrication. Thus, the new center would get an enormous unprecedented upstart with 117 representative major equipments, worth ~$50 million, already in place. (https://cinap.ibs.re.kr/html/cinap_en/)

(Research trends) After experimental realization of the single-atom-thick carbon layer, graphene, various thin-layered crystals have been studied at nanoscale. A group of new quantum materials have been extensively studied due to their unique physical properties in contrast to their bulk part. Nowadays the research in quantum materials has been extended to a variety of areas of science and technology, which settled as one of the big research fields. The library of quantum materials covers most classes in condensed matter physics: metals, semiconductors, insulators, superconductors, and magnets. The quantum materials have uncovered emerging quantum mechanical phenomena such as quantum transport properties including the quantum Hall effect, Klein tunnelling, topological properties, and valley properties. Over the past decade, a few new materials have been discovered and various methods on device fabrication were rapidly developed to control the emerging physical phenomena out of the quantum materials. This research area is keep emerging and expanding so that even more and more intriguing and surprising phenomena, for example superconductivity from magic angled twisted bilayer graphene, Berry curvature and pseudospins, were unveiled. Not only studying the fundamental physics, industrial applications of quantum materials are also pursuing in worldwide.
The realization of unconventional atomic assembly via the control on nanometer scale will broaden the horizon of research activities and lead to the observation of exciting phenomena of fundamental importance. One striking aspect of these activities would be the decisive role the theory part would have to play. New quantum materials are not just discovered serendipitously but designed theoretically. Of course, at the current level of computation capability, the materials design would not be simple; nevertheless, this is obviously the direction for a cutting edge center on nanophysics such as an IBS center to head towards.

(Necessity for IBS) The research in quantum materials requires close collaboration of expertise from a broad research area. For the fabrication and characterization of quantum materials, the technique should be newly developed or optimized for them. Furthermore, since its diversity, each class of quantum materials requires a different approach to be properly investigated. This implies every step for the research in quantum materials requires expertise in a different field. The close interaction between IBS members will be generated a synergic effect on the research. To be successful, the fabrication and characterization should be corroborated by frequent interaction and feedback from each other. Researchers equipped with various quantum material synthesis equipment, transfer and stacking alignment process equipment, advanced quantum physical property measurement equipment, and expertise synthesized in the centre measure the electronic structure of Hamiltonian engineering in quantum materials through synergistic research and it will secure the know-how to control up to atomic resolution. Through this center, we will secure quantum computing know-how by establishing the principles and mechanisms of quantum transport phenomena related to new horizons like straintronics, twistronics, and valleytronics beyond spintronics, it is expected that the joint utilization of research equipment will lead to technologies to understand and control various chemical and biological reactions.

## 3) Experimental physics – Rare isotope (RI) sciences

### ■ Nuclear Physics *(Designated in 2015, rev. 2021)*

Nuclear physics is one of the key fields in physics. It has been played a crucial role in understanding not only the nature at the subatomic level but also the various astrophysical objects. The major goal of the new rare-isotope (RI) beam facility, RAON, at IBS is the investigation of the structure of the unstable nuclei and the fundamental interactions among their constituents in highly compressed environment as well as vacuum. The most interesting subjects that can be explored by the RI beams can be summarized as following:

- Nuclear structure: Structures of the newly discovered rare isotopes, exact location of the drip lines, new magic numbers, and tensor force
- Nuclear astrophysics: Origin of the elements, nuclear reactions in the r- & rp-processes, evolution of stars, elemental abundance ratios in stars, and structure of neutron stars
- Nuclear reaction: Equation of state for isospin asymmetric nuclear matter (or symmetry energy), level densities of nuclear matter, fusion, fission, direct reactions
- Theory: Fundamental symmetry, framework of describing structures of nuclei and their interactions, equation of state (EOS) of dense matter, and reaction mechanisms

The research subjects, which are not necessarily limited to the above areas, are quite extensive, and the organized efforts are required. As a starting point, the Center for Exotic Nuclear Studies (CENS) was launched in 2019 as one of the IBS research centers dedicated to the nuclear structure and astrophysics mostly at low energies. It comprehensively covers the various subjects on the nuclear structure and nuclear astrophysics. However, obviously just a single center cannot cover all interesting research topics that can be explored by RAON. To maximize the usage of the world-frontier RI accelerator facility RAON, the additional IBS center dedicated in large to the nuclear matter, particularly, at high baryon densities is desirable.

Recently, the gravitational wave generated during the merging process of the two neutron stars was detected. Then, this enormous process has gained a lot of attention as one of the potential sources for elements heavier than Fe. Since the core of the neutron star consists of the compressed nuclear matter, the strong interaction at the microscopic level in dense-matter environments is a key to understand the heavy-element production in the astrophysical processes.

In addition, the symmetry energy in the equation of state (EOS) of nuclear matter at densities larger than the saturated value is important to investigate not only the neutron stars, but also other objects like supernovae, proto-neutron stars, X-ray bursters, etc. With intense efforts so far, the symmetry energy function at or below the saturated value can be determined rather accurately by now. However, the experimental and theoretical studies of the symmetry energy at supra-saturation densities is being just started with advent of the various modern RI beam accelerators, such as RAON, FRIB, RIBF, and FAIR that can provide the exotic rare isotope beams with beam energies of several hundred MeV per nucleon. It is timely to initiate this effort to lead the field in mind the schedule for the completion of the high-energy section of RAON in around 2027.

## ③ Chemistry

### ■ Experimental and theoretical chemical physics *(Designated in 2017)*

(Research trends) Chemistry is a central science that bridges various fields, including biological and materials science. Chemistry can play a role as a central science because the principles of chemistry are based strictly on physics, such as quantum mechanics and statistical thermodynamics, and are directly applicable to biological and material sciences. Any paradigm shift in physics has made, therefore, profound impacts on every aspect of chemistry. For example, the advent of quantum mechanics in the early twentieth century changed drastically how chemists understood molecules and atoms. At the same time, new materials (such as magnetic metal oxides) synthesized by chemists in the 21st century has inspired physicists. Chemical physics – an interdisciplinary subject of chemistry and physics – is, therefore, a passageway where recent advances in one field may lead synergistically to unexpected outcomes in other fields. In particular, a major challenge in chemical physics is the development of theoretical and experimental methods to understand complex materials and biological systems, and elucidate the interaction between light and matter (e.g. the electronically excited states).

(Necessity for IBS) The Center for Experimental and Theoretical Chemical Physics aims to establish new theoretical and experimental paradigms, in light-matter interactions, control of chemical reactions and complex systems. Therefore, spectroscopy (NMR, EPR, vibrational, single-molecule, etc.), microscopy (Cryo-EM, force, near field optics), scattering (X-ray laser) and computer simulations (DFT, multiscale modeling) should be the main tools of the Center. Synergistic collaborations among groups in the Center will facilitate the development of a new generation of theoretical and experimental methods. The researches in the Center will provide a strong foundation for understanding chemical and biological processes.

(Key research contents) The research of the Center will focus on the following areas: 1) Multi-technique structural and dynamic characterization; 2) Precision measurement of complex chemical and biological processes; 3) Computational chemistry; and 4) Non-equilibrium statistical mechanics for chemical and biological processes. Multi-technique structural and dynamic characterization should cover broad spatiotemporal scales of complex materials and biological systems, thus providing a new set of physical insights. Developing the next generation precision measurement technique should be an issue of importance in physical chemistry. It will be a basis to elucidate the exact mechanisms of complex processes, such as response and feedback in a biological process, and synthesize highly functional molecular systems. Computational chemistry is quite versatile and lies in between experiments and theories. Thanks to recent impressive developments in computers and algorithms, computational chemistry may cover almost every aspect of chemical systems from small organic molecules to macroscopic, biological, and materials systems. This puts computer simulation on equal footing with experiments and makes it an indispensable tool. Recent studies on biological and chemical processes revealed that such complex systems are far from being in equilibrium states, illustrating why equilibrium thermodynamics often fails to describe such processes. Developing theoretical and computational tools to elucidate such non-equilibrium processes should provide opportunities for understanding complex systems better.

## ■ Chemical biology *(Designated in 2017)*

(Research trends) Chemical biology is a field of science that aims to understand the underlying mechanism of biological systems with molecular precision through the integrated approaches of chemistry, biology, and allied disciplines. The molecular-level understanding and controlling of biological processes can lead to the selective manipulation of biological phenomena, especially those related to human diseases. Cutting-edge research in chemical biology is a promising and essential area in biological science, and serves as a powerhouse of knowledge-based discovery of novel medicines, early diagnosis, and innovative advances in research tools at the interface between chemistry and biology. Related research fields include bioorganic chemistry, target identification/engagement, fluorescent live-cell imaging, drug discovery, phenotypic screening, bioorthogonal chemistry, and related disciplines.

(Necessity for IBS) The Center for Chemical Biology aims to understand the fundamental mechanisms of human diseases at the molecular level, and use this knowledge to control biological processes. This level of understanding is not possible without the integration of cutting-edge technologies, including molecular biology, chemical proteomics, molecular diversity, high throughput bioassays, high content phenotypic screening, fluorescent bioimaging, target identification/validation, etc. The close interactions between the research groups with different disciplines will generate a synergistic breakthrough in the mechanistic understanding of mysterious biological systems, along with: the discovery of novel first-in-class therapeutic agents, the platform development for early diagnosis, and the identification of biomarkers for human diseases. Therefore, it is essential that the Center for Chemical Biology should be composed of multiple principal investigators operating mutually complementary research systems.

(Key research contents) The research topic of this Center includes 1) Chemical tools modulating biomolecular interactions in human and model organisms; 2) Chemical tools for elucidating allostery and molecular machinery; 3) Chemical toolbox for post-translational modification and epigenetics; 4) Novel technical platform for bioimaging and biomedical research; and 5) Chemical proteogenomics. Chemical biology, combined with rigorous molecular cell biology, will provide a unique opportunity for developing new therapeutics and biomarkers of human diseases. Based on the fundamental understanding of molecular mechanisms of human diseases, the well-established rational drug discovery approach will be applied to facilitate the development of novel first-in-class therapeutics in human diseases. Using novel chemical biology technology and their integrated platform, the Center for Chemical Biology should provide opportunities for novel findings and application in treating human diseases.

## ■ Molecular electronics *(Designated in 2017)*

(Research trends) Molecular electronics is an interdisciplinary research field for the design and applications of molecular building blocks for electronic devices. After the discovery of electron-conducting polymers, various organic semiconducting materials have been developed for the design of efficient molecular electronic devices to overcome the limitation of silicon-based technology. Following the progresses in microscopic observation techniques, molecular electronics achieved significant improvements as experimental field to study charge transport phenomena at the molecular level. The ultimate goal of molecular electronics would be the fabrication of molecular level electronic devices with high efficiency.

(Necessity for IBS) The Center for Molecular Electronics aims to accomplish the fundamental understanding of the molecular level electronic properties in the molecular build blocks of organic electronic devices. These include organic photovoltaics, organic light-emitting diodes, field-effect transistors, photodiodes, etc. Although various semiconducting organic materials have been explored for the fabrication of organic electronic devices, we have not fully understood the molecular level electron transduction processes yet. Therefore, scientists carry out trials and errors to improve the efficiency of the electronic devices. The fundamental understanding of molecular-level electronic behavior will bring a breakthrough in the field of molecular electronics.

(Key research contents) The Center's research will direct its efforts on 1) Fundamental understanding of energy, electron, and hole transfer process in biomimetic architecture; 2) Design of semiconducting organic molecules and molecular devices for sustainable energy; 3) Molecular assemblies for advanced organic electronic devices; and 4) Molecular simulation study for efficient electronic device fabrication. The study on biomimetic architecture will provide new insight into the discovery of advanced electronic devices. Because the organic electronic devices possess potential solutions for energy and environmental crises, the fundamental understanding of molecular electronics and rational design of semiconducting organic molecules has great value. Additionally, the fine control of molecular level self-assemblies will be an important project for the fabrication of well-defined architecture. The molecular simulation study will help the rational design of semiconducting organic molecules and the understanding of molecular-level self-assembly phenomena. Through the collaboration of the above research topics, the Center should provide great advances in the field of molecular electronics.

## ■ Next-generation synthesis of complex molecules *(Designated in 2017)*

(Research trends) Defining the frontiers of organic chemistry, the synthesis of complex target compounds of known or designed molecular structures, starting from available small molecules, is one of the most basic and essential tasks. In the 20th century, the art of organic synthesis, total synthesis in particular, improved to impressively high levels of sophistication: even seemingly impossible molecules could be constructed in laboratory. Now in the 21st century, new strategies are clearly needed to achieve 'ideal' syntheses. These would allow the construction of linked small molecules, with a sequence of successive reactions that involve no intermediary re-functionalization, and lead directly to the target structure. Such a synthesis would be the most economical: it would provide large quantities of highly complex molecules with a minimum amount of labor and material expenses.

(Necessity for IBS) Success in the ideal synthesis of complex molecules requires a group of experienced synthetic professionals, sufficiently long research periods, and stable research funds. Young synthetic chemists generally have unstable social positions under current research environments, and so they are commonly reluctant to start their research careers in the synthesis of complex molecules, which is viewed as "a risky business." Aware of the ultimate challenge to achieve such ideal syntheses, the Center for Next-Generation Synthesis of Complex Molecules would benefit from IBS-sponsorship.

(Key research contents) The ideal synthesis of complex molecules, especially total synthesis, is a starting point for the development of novel synthetic strategies and methodologies, including new reactions and reagents. The research in the Center will also establish computer-aided synthesis design and automated synthesis by synthesis machines. Although synthesis has to be viewed as an art and a science that needs to be advanced for its own sake, the Center for Next-Generation Synthesis of Complex Molecules would leverage the power of the ideal chemical synthesis to address problems in catalysis, natural product assembly, drug discovery, and chemical biology. The Center will also investigate the naturally evolving pathway of organic molecules from the rudimentary building blocks of life to the more mature and essential components of life from a synthetic chemist's perspective. A systems chemistry approach may eventually unravel the origin of life from the standpoint of molecules. In order to serve humanity optimally and to fully exploit its power, the next-generation synthesis can help push the limit and shape the new frontiers in biology, physics, biotechnology, and nanotechnology: multiple collaborations can be forged with an ample variety of desired materials.

## ■ Chemical neuroscience *(Designated in 2019)*

(Research trends) How does the brain work? To address this, understanding chemical signals that mediate and/or modulate neuronal communication and their relationship with behavioral changes in animals is obviously necessary. However, last century's efforts to answer this question have been largely undertaken via physiological, cell biological, molecular biological, and more recently genetical approaches. This is ironical, given that most of synaptic transmission and neuromodulation is chemical in nature.

Another emerging neuroscience problem is neuroinflammation, which is related to all the neuronal disease. The imaging, diagnosis, and treatment of neuropathology using chemical tools compose a fundamental, and at the same time, clinically applicable research field.

Obviously, this quest cannot be done by chemists alone. A successful program would need, among others, neurobiologists who understand the neural systems, engineers to build sensors that translate chemical signals to tangible and quantifiable readouts, computational biologists who can model these complex interactions, and medicinal chemists to develop new therapeutics.

(Necessity for IBS) This new area should benefit IBS, given that 1) chemical neuroscience itself is new, and 2) synergistic with existing IBS researches. It could provide chemogenetic tools and probes to the Center for Cognition and Sociality, the Center for Synaptic Brain Dysfunctions, the Center for Neuroscience Imaging Research, and the Center for Nanomedicine.
(Key research contents)

1) Chemical probes (molecular sensors or cellular highlighter) that reveal cellular identities and processes within the brain, such as calcium indicators, voltage indicators and sensors for synaptic transmission;

2) Developing chemogenetic tools that can be used to control and investigate cell signaling;

3) Imaging probes for neuro-inflammation or immunological cells, for diagnosis and disease monitoring of neurodisease;

4) Using genetically encoded unnatural amino acids in live brain cells and even organisms, to investigate biological processes in the brain.

■ **Sustainable chemistry** *(Designated in 2019)*

(Research trends) The traditional research in chemical science has been initiated from the desire for understanding the nature of matter and its changes. The overall outcome obtained from the endless efforts and discoveries made by chemists over the last several centuries has not only widened mankind’s understanding of mother nature, but also enabled all human beings to live their lives in unprecedented prosperity. However, taking advantage of those discoveries without serious consideration of the malicious side effects on our environment has put our Earth in unexpected sufferings, such as global warming, air/water pollution, and ecosystem disturbance caused by mass-produced chemical products. Fortunately, a few chemists became seriously aware of the problem several decades ago and started to advocate the idea of the so-called “green chemistry” or “sustainable chemistry.” Research efforts in sustainable chemistry have been concerned with reducing chemical wastes, employing energy-efficient processes, and using renewable material feedstocks and environmentally benign substances. However, most of the research efforts in this field so far have been made from an engineering perspective, rather than from a scientific perspective, meaning that the most efficient processes have been dragged from the existing knowledge and technology. To make this sustainability-related field truly sustainable, breakthrough innovations based on new scientific discoveries are highly desirable.

(Necessity for IBS) Research in sustainable chemistry inherently requires collective efforts from various fields, including synthetic chemistry, analytical chemistry, physical chemistry, and biochemistry. Strong synergy is expected from the collaboration between small expertise groups aiming to the same goal: the “exploration of sustainable chemistry”. There will be several chances to encounter beneficial discoveries for human beings, because the research is motivated by the curiosity underlying the righteous motto, “Save the Earth”.

(Key research contents) The Center for Sustainable Chemistry should explore the following research subjects

1) New strategies for atom economic synthesis: design and synthesis of new efficient catalysts, discovery of new chemical reactions minimizing the use of reagents and the production of side products;

2) Environmentally benign chemistry: reactions in water, light-driven reactions, reduction of carbon dioxide, waste minimizing catalysts, electrosynthesis;

3) Energy harvest from the Sun: efficient photovoltaic cells, discovery of new photo-reactions, artificial photosynthesis;

4) Development of bio-mimic systems: bio-inspired smart materials, eco-friendly materials;

5) Materials from renewable resources: new synthetic methodology for polymers and other materials from biomass.

## ④ Life sciences

### ■ Aging biology *(Designated in 2019, rev. 2021)*

(Research trends) With the discovery of effective longevity genes and their networks, expectations for retarding the aging process are increasing steadily. Simultaneously, humans are now facing a new and fundamental dilemma due to the manifestations of various irreversible age-related diseases, which prevent the increase in healthy life expectancy, thus burdening healthcare costs worldwide. Scientists are now searching for fundamental mechanisms for the aging of organisms utilizing various models. They employ comprehensive modern scientific knowledge and technologies in genetics, genomics, proteomics, and molecular and cellular biology on immunity, nervous system, metabolism, and rejuvenation by stem cells. While the complicated system of human aging processes prevents the immediate translational application of the results obtained from other model systems, the acquired scientific discoveries and profound understanding of the diseases related to aging would provide an opportunity for intervening in the aging process.

(Necessity for IBS) Research on aging has been vigorously pursued by individual scientists in the past few decades. Since the vast areas of biological processes and diseases are related to the aging process, scientific pursuit at individual levels with limited resources and expertise has restricted the establishment of domestic research infra of the currently emerging and globally developing research field. Studies on the aging process in animal model systems and humans, molecular and cellular biology, genetics, genomics, and age-related diseases require vast amounts of time, manpower and financial resources; thus, it is necessary to initiate basic animal aging studies at the scale of IBS Research Centers. The IBS Center for Aging Biology needs to become the hub that connects basic scientists and clinicians and aims to develop a better understanding of human aging using various model systems as well as multidisciplinary approaches.

(Key research contents) The research will cover molecular and cellular biology, genetics, physiology, and clinical medicine, focusing on human aging and age-related pathologies to understand the human aging process.

- Molecular and cellular biology studies will include cell senescence and death, the cellular microenvironment and its effect on age-related tumors, age-related protein homeostasis and degradation, and telomerase biology.
- Genetic studies on longevity in various model systems (Caenorhabditis elegans, fruit flies, mice, zebrafish, monkeys) and humans are also required. In particular, discoveries of novel genes and their networks that affect human longevity will open a new area of research and therapeutic opportunities. The genomics, gene expression, functional genomics, and genomic instability of aged animal model systems will provide a comprehensive understanding of the human aging process at the chromosomal level. In addition, epigenetic studies are required to expand the scope of aging research to environmental, external, and imprinting factors.
- Since the systemic metabolism changes vastly during the aging process and may result in various age-related metabolic diseases that affect life span, the molecular and genetic aspects of caloric restriction, oxidative stress, mitochondrial function, hormonal responses, microbiotal changes, skeletal muscle deterioration(sarcopenia), etc. need to be pursued.
- Studies on the phenomena of immunoscence in the adaptive and innate immune system, autoimmune diseases, and age-associated chronic inflammation, employing various animal

models and human will be important to understand the aging process.
- The program of regenerative biology, including stem cell renewal and differentiation, and anti-aging biotechnical applications, will translate basic research to clinical approaches.

## ■ Developmental cell biology *(Designated in 2017, revised in 2021)*

(Research trends) How does a single cell develop into a multi-cellular and differentiated organism? What controls organ regeneration? How can a skin cell become a nerve cell? These kind of questions in mammalian developmental biology are still to be answered. Revealing the identity of a cell and its time-dependent regulation (chrono-developmental biology) are fundamental inquiries of biological sciences. Although all cells of an organism have identical copies of genetic information, it is their different developmental programs that lead to their distinctive developmental fates. Furthemore, developmental fates are affected by the spatio-temporal control of transcription , differentiation, epigenetic regulation, chromosome dynamics, etc. Although Gurdon and Yamanaka were awarded for Nobel Prize of Physiology or Medicine in 2012 for their discovery of reprogramming of mature cells into pluripotent cells, some fundamental concepts of cell reprogramming are still remianed to be solved. Combining with the recent development in single-cell omics, data science and imaging technologies, essential questions of how a single cell develops into a whole organism and how life is made could be further pursued.

(Necessity for IBS) One should be asking such bold questions as follows at the IBS Center for Developmental Cell Biology (DCB). 1) Unveiling transcriptional and epigenetic control of stem cell maintenance and differentiation; 2) Symmetric and asymmetric division of cells in development; 3) Genotype-phenotype challenge using model animals; 4) Understanding development in time and space; 5) Tracing the development of a cell using multi-omics at the single cell level and use of state of the art imaging techniques.

(Key research contents)

- How the information coded in the genome leads to the specification of physical characteristics may be answered through combining multiple disciplines including developmental biology, single-cell omics, imaging cell biology techniques, integrative data science, etc.
- Elucidating the stemness is an important issue to understand how cells constitute tissues, and how cells grow and differentiate. Using genetically modified animal models and adopting novel stem cell technologies, the Center is expected to provide opportunities for; understanding how genetic programming and reprogramming turns on cell differentiation, how stemness is maintained, and finally how these understandings could be implicated in in treating human diseases.
- Single-cell omics, including RNA sequencing incoportated with recently developing single cell DNA and protein sequencing technology will give insights of the spatio-temporal regulation of cellular function in development. When combined with the use of high-resolution imaging techniques, this multi-omics approach will open a new horizon in the field. It and provide new therapeutic clues to dysfunctional developmental disorders in humans.
- The development of an organism requires 'time-dependent changes' in the fate and location of every single of its cells, which result in organogenesis and regional specification of its body

parts. How this whole process is coordinated and controlled in 'time‘ is unclear: there might be a 'master clock' able to communicate with all the cells that controls the course of complicated events during development. Elucidating temporal coordination of each body part and related topics will offer a chance to deepen our understanding of the time-dependent changes of anatomy and physiology.

## ■ Integrated omics *(Designated in 2017, revised in 2021)*

(Research trends) With the maturation of individual omics fields, such as genomics and proteomics, integrated omics has emerged as a next-generation approach for holistic understanding of disease-related cellular events. Several representative consortium projects, such as The Cancer Genome Atlas (TCGA), Human Microbiome Project (HMP), Brain Initiative, Precision Medicine Initiative (PMI), and LifeTime Initiative, have employed integrated omics approaches combining multiple types of omics analyses. Two cardinal pillars of the integrated omics analysis are 1) comprehensive analyses that generate system-level data in cells, tissues, or organs relevant to dynamically changing multiscale cellular processes; and 2) computational methodologies for integrating different types of individual omics data to generate new hypotheses regarding fundamental biological and medical questions. Despite recent advances in omics technologies and data analyses, there are still significant needs for new omics technologies and data integration methodologies. Recently, longitudinal medical and health (dietary data, family history, exercise data, etc.) records of large patient cohorts are analyzed together with various omics data using statistical or AI methods, linking integrated omics with diagnosis and therapy. This line of research aims to address challenging biological and medical questions by developing creative integrated analysis approaches for diverse omics data and big medical/health records.

(Necessity for IBS) Owing to the efforts of diverse centers and research projects for the past 20 years, data generation technologies and data analysis methods for individual omics (genomics, proteomics, metabolomics, etc.) are now well standardized. However, compared to individual omics, an integrated analysis of multiple omics datasets, possibly together with big longitudinal medical/health records, requires new technologies and methodologies spanning such fields as genomics, proteomics, informatics, AI, phenomics, biochemistry, in vivo and clinical models, technology development, and medical/health records. Examples of such technologies include single-cell level proteomics for intracellular signaling networks and interactomics for decoding dynamic evolution of interaction networks. Accordingly, no single researcher can handle this research in full spectrum, and tight collaborations among researchers with diverse expertise are essential for the success of the perspective Center for Integrated Omics.

(Key research contents) The new IBS center should aim to solve challenging biological problems that can lead to innovative and transforming outputs, but cannot be answered effectively without integrated data analysis. A detailed integrated analytical approach should be designed to effectively answer such biological questions. Then, the methodology to integrate multiple types of global biological data and/or longitudinal medical data should be clarified. These activities would involve tight collaborations with engineers, bioinformaticians, and/or clinicians. Finally, potential impacts of research outputs for the advancement of biology or medicine should be clearly addressed.

■ **Molecular synthetic biology** *(Designated in 2017, revised in 2019, 2021)*

(Background) While studies on the molecular complexes or systems (e.g., protein complex, superenhancer module, regulatory RNA complexes, etc.) governing cell growth, differentiation, transformation, and death have been heavily investigated, their molecular and functional bases in association with many life-threatening diseases remain to be understood. Recent progresses in molecular and chemical technologies, such as gene editing (e.g., CRISPR), high-resolution imaging (e.g., CryoEM), chemical genetics, omics technologies, and synthetic biology, provide an unprecedented opportunity to tackle various questions regarding the molecular systems as well as to reprogram the operation of the systems to drive them into desired states. Orchestrating these emerging probing and control technologies to unveil the operation principles and control strategies for key molecular systems is a great challenge at the moment. This research is designed to address challenging biological or medical questions by developing creative approaches integrating diverse probing and control technologies.

(Necessity for IBS) The Center for Molecular Synthetic Biology (MSB) aims to unravel and control key molecular systems in various biological phenomena by effectively integrating diverse probing and control technologies employing model organisms, such as mouse, Drosophila, C. elegans, yeast, etc. The Center will be composed of groups using different disciplines with the common aim to understand the fundamental questions unanswered. The close interactions between the groups with distinct research expertise and model organisms will generate a synergistic melting pot that encourages novel ideas and technologies and produce innovative research outputs. The Center can serve as a liaison of other IBS Centers and domestic institutes as well due to its unique specialization for probing and controlling various molecular systems in diverse model organisms. Such interdisciplinary research Center will constitute a collaborative cluster that promises the emergence of novel techniques and fields.

(Key research contents) Key questions related to challenging and unsolved biological and medical problems should be first addressed, followed by a proposal of innovative and transforming outputs. Detailed integrated approaches including developed or existing multiple types of technologies and methodologyies should be designed and employed to effectively answer such biological questions. These activities would also have to involve tight collaborations with engineers, bioinformaticians, synthetic biologists, and/or clinicians. Finally, the potential impacts of the research outputs on advances or innovation of biology or medicine should be clearly addressed.

■ **Phytobiology** *(Designated in 2019, revised in 2021)*

(Research trends) Plants, as sessile organisms, show remarkable developmental plasticity during their growth/development to adapt in response to their surrounding environmental changes. How plants perceive and respond to the continuously changing environmental conditions is a critical fundamental question in plant biology. The scientists in basic plant biology, working with modern model organisms like thale cress, focus on the signaling networks of light and temperature (the two most important environmental factors), phytohormone signaling network, regulation of plant vegetative development, regulation of plant reproductive development, and plants' response to the environment. In plant genetics and biotechnology, recent advances in

CRSPR tools allow gene editing in plant organelles, including mitochondria and chloroplasts. In addition, the domestication of wild plants is another field of emerging interest. The selection of identical traits during domestication of different species strongly indicate the presence of domestication traits and corresponding domestication genes. Once candidate genes are identified, they can be targeted by CRISPR-based genome editing tools and the traits of wild plants would be tamed.

(Necessity for IBS) The Center for PhytoBiology Research (CPBR) aims to increase our understanding of how plants modulate their growth and development, which will form an important foundation for long-term global sustainability. For competitive science in phytology field, the study requires a coordinated effort among scientists with a broad spectrum of expertise, including plant molecular genetics, plant developmental biology, plant tissue culture, genomics, phenomics, metabolic analysis, and genome editing technology, as well as related facilities.

(Key research contents)

- Temperature signaling network of plants: Temperature changes often perturb plant ecosystems by altering developmental program, thereby affecting the optimal timing of flowering for successful reproduction. Understanding and dissecting the molecular mechanisms underlying the ambient temperature response in plants growing under continuously changing temperatures is very important.
- Light signaling network of plants: Plant photoreceptor systems play critical roles in decoding the light-produced information, and plants then integrate this with other information coming from systems detecting other endogenous/environmental factors. Close collaboration between plant genetics and physics will provide new tools customized to study plant responses to light.
- Hormone signaling network of plants: The plant integrates environmental cues into intrinsic developmental programs (i.e. phytohormone signaling networks), to optimize its growth and development. Clarifying these complex interactions is a prerequisite to elucidate the signaling networks of phytohormones.
- Regulation of plant vegetative development and reproductive development: Identifying the factors that regulate vegetative growth at the biochemical and molecular levels and deciphering how these factors coordinate the changes in vegetative tissue development are especially important to increase body mass, photosynthesis, and nutrient uptake. Likewise plant sexual reproduction is a fundamental process that is critical for both human survival (via food production) and the maintenance of diversity in flowering plants. Plants monitor and integrate environmental cues to optimize their survival and reproduction including flowering time, floral patterning, fertilization, and gametophyte/seed development. The importance of fine-tuning plant hormone production, epigenetic reprogramming, signal transduction, and in situ quantification of metabolite levels should be also investigated.
- Response to stresses: Plants continuously face abiotic/biotic stresses, such as pathogens. Improving crop yields, both in magnitude and consistency, will require intensive studies on stress-responsive growth factors, the regulation of their effectors, as well as their secondary signals. Translating the knowledge gathered from model plants to crop plants will be also necessary for potential agricultural applications. Investigating the roles of critical modulators in abiotic and biotic stress tolerance is important for the development of crop plants tolerant to a broad range of unfavorable environments.
- Plant domestication by design: The project will start by identifying wild plant species that might

be developed as new crop species and examining their physiology and development. Then, their metabolites must be cataloged, their interactions with pathogens and environmental signals must be determined, and target traits must be identified. Once target traits are identified, their genomes have to be sequenced, their pant tissue culture and genome editing methods have to be developed, and breeding programs have to be established. All these activities would require tight collaborations among experts not only in plant sciences but also in bioinformatics and breeders.

■ **Integrative systems neuroscience** *(Designated in 2017, revised in 2021)*

(Research trends) A major hurdle in understanding the neural basis of brain functions is the complexity of the brain. The human brain contains trillions of interconnected cells and possibly more than 1,000 types of neurons. Traditional systems neuroscience aims to understand how emergent properties of such complex neural circuits give rise to diverse brain functions by monitoring and manipulating ongoing neural activity in intact organisms. Owing to technological advances in molecular biology, it is now possible to obtain the whole transcriptomic and proteomic data of neurons at the single-cell level, and analyze them to label and control any particular group of neurons and their connections for circuit mapping of specific brain functions. In addition, real-time and high-resolution monitoring of neuronal activities of the brain by advanced imaging and neurophysiological approaches are becoming increasingly feasible. These comprehensive dissections of the brain from gene to function require systematic collection of a large amount of data and sophisticated integrative analysis of these data, namely brain big data analysis. An example is the Brain Initiative Project, an ambitious US plan to better understand and cure the brain, where big data on thousands of individual brain cell types and their wiring and firing patterns are being gathered and analyzed using advanced imaging and computational technologies. Many world-class research centers (e.g., the Allen Institute for Brain Science and Janelia Research Campus) also investigate specific characteristics of each neuronal cell types, including molecular composition, morphology, synapse profiles, and firing patterns.

(Necessity for IBS) There are excellent neuroscientists in Korea specialized in genomics, transcriptomics, proteomics, circuit mapping, neurophysiology, and computational modeling. However, a concerted effort to integrate these approaches for comprehensive understanding of brain functions in terms of molecules, synapses, and circuits, is lacking. Given the immense complexities and great potential of the brain, future IBS centers would have to take crucial steps to explore the fundamental aspects of the brain complexity, for instance, by focusing on specific organisms, brain regions, and brain functions. A few examples of such brain functions include attention, sensory integration, memory, executive function, and emotional regulations. These explorations would be greatly accelerated by large-scale systematic collection and analysis of global data on neuronal and circuit functions at genomic, molecular, synaptic, neuronal, and circuit levels.

(Key research contents) Functional connectome mapping of the brain would involve molecular profiling of the neuronal cell types (via single cell-level transcriptomics/proteomics), morphological profiling of neurons (4D morphology, neurite branching, and synapse distribution), functional profiling of neurons (intrinsic neuronal excitability and firing), neuronal circuit mapping, and computational modeling. For big data analysis of the brain in health and disease, future IBS centers would have to systematically collect and analyze activity profiles of specific neuronal cell types and related these to molecular and circuit mapping data. The centers also develop and use advanced tools/platforms for integrative data collection and analysis. These activities would also have to involve tight collaborations between basic neuroscientists, engineers, and clinicians.

## ⑤ Science of global and regional environmental changes

### ■ Coastal hazards *(Designated in 2012, rev. 2021)*

- Assessing coastal hazards induced by changes in climate, sea level, ocean acidification or triggered by geological processes (e.g. earthquakes)
- Studying the physical and biogeochemical state of the ocean and its anthropogenic drivers using state-of-the art monitoring capabilities and numerical models
- Investigating the influence of sea level rise on coastal processes including erosion and the interaction with groundwater hydrology
- Including but not limited to the above areas of study

### ■ Air pollution and atmospheric chemistry *(Designated in 2021)*

- Studying sources of air pollution, transport mechanisms, relevant chemical reactions
- Monitoring and predicting air pollution with ground-based systems, aircrafts, satellites, and numerical models
- Investigating the impact of air-pollution on human and animal health
- Including but not limited to the above areas of study

### ■ Geobiology *(Designated in 2021)*

- Studying the co-evolution of life and climate on our planet
- Assessing the long-term planetary habitability and biological resilience through understanding of geosphere/biosphere interactions
- Understanding and modifying plant responses to increasing CO2 concentrations with relevance for global food security
- Developing mathematical models to understand and simulate evolutionary biological processes in changing environmental conditions
- Including but not limited to the above areas of study

### ■ Climate and health *(Designated in 2021)*

- Quantifying climate change effects on infectious and parasitic diseases through epidemiological work, advanced statistics and computer modeling
- Assessing risks of extreme heat on human and animal bodies (e.g. lifestock), including heat stroke, kidney failure etc.
- Understanding the impact of climate change on regional habitats of disease vectors
- Determining the impacts of climate on pollen production and allergic diseases
- Including but not limited to the above areas of study

## ⑥ Interdisciplinary

### ■ Science of imaging *(Designated in 2017, revised in 2019)*

(Research trends) The advance of imaging science has been essential for the advance of science itself. For instance, telescopes, microscopes, and spectroscopes have revolutionized our understanding of the universe, living organisms, and the quantum-world, respectively. A recent creative combination of microscopic and spectroscopic techniques has created powerful spatial images at the molecular level. This unprecedented high spatial resolution, however, was achieved at the expense of time resolution. The next revolution in scientific imaging is anticipated in the area of molecular dynamics with both high spatial and time resolutions, which is expected to bring about breakthroughs in key systems, such as solar energy harvesting in artificial photosynthesis. High-resolution imaging of biomolecules, cellular architecture and tissue will also revolutionize molecular cell biology, medicine, and brain science. The recent success of Cryo-EM in protein imaging needs to be extended to other key biomolecules and cellular structures. A new imaging technique would be desirable for miRNA – short regulatory RNAs that control the expression of 30% of protein-coding genes at the post-transcriptional level. Expression of miRNAs should be tightly regulated, and its dysregulations are related to cellular malfunctions and numerous diseases, making the accurate profiling of miRNA expression extremely important in both biology and medicine. Due to their small size, however, detection of miRNAs presents special challenges, making conventional techniques used for larger RNAs unsuitable in miRNA detection. Novel miRNA imaging technology will open a door to deep understandings of how key biological processes such as development and learning/memory are regulated by miRNAs.

(Necessity for IBS) IBS aims to focus on fundamental researches in selected areas that can make a high impact both intellectually and practically. One of the prime examples would be imaging surface dynamics of redox processes in heterogeneous catalysts with atomic resolution. Another example would be the development of efficient and reliable miRNA imaging and profiling methods. Creating a world-class IBS Center for the Science of Imaging, tackling critical problems in energy sciences, molecular biology, and neurosciences, will help meet next-generation scientific challenges and contribute to enhancing the international visibility of IBS.

(Key research contents) The perspective Center will focus on one or more of the following areas. 1) Real-time luminescence/absorption spectroscopic and magneto-optical spectroscopic imaging of catalysts and electronic devices with atomic resolution; 2) Cryo-EM (single-particle cryo-electron microscopy) and Cryo-ET (cryo-electron tomography) for high-resolution and dynamic structure analysis of biomolecules and cellular machinery; 3) miRNA imaging and profiling with cellular resolution at the tissue level; 4) Liquid cell electron microscopy for the study of the dynamics of biomolecules and their complexes in real-time; and 5) Other emerging techniques, such as genomic, transcriptomic, and proteomic imaging with subcellular resolution by far-field, label-free spectroscopic imaging of single molecules in ambient condition.

## ■ Biophysics and biochemistry of membrane proteins *(Designated in 2019)*

(Research trends) Approximately 40% of all cellular proteins reside in the non-aqueous environment of lipid membranes, where they play critical roles in metabolic functions and regulating the transfer of information and materials into and out of the cell. Membrane proteins govern such processes as nutrient uptake, drug efflux, respiration, sensory physiology, immunity, and neuronal communication, to name a few. It has been widely acknowledged that membrane proteins are also central components in numerous disease states and host-pathogen interactions. However, due to their hydrophobic environment, isolation and characterization of their structure and function remain extremely challenging.

(Necessity for IBS) The Center for Biophysics and Biochemistry of Membrane Proteins aims to study molecular mechanisms and biophysics of membrane proteins, both 1) using electron microscope, X-ray, NMR, laser spectroscopy, label-free optical and vibrational microscopy, and 2) developing novel techniques. An ideal complement to the experimental studies is to develop theoretical and computational methods such as quantum chemistry, statistical mechanics, and classical/quantum/hybrid molecular dynamics simulation, that are useful for gaining a detailed understanding of the underlying principles and mechanisms.

(Key research contents) The research area of the Center includes the development and/or application of (1) Cryogenic electron microscopy and tomography; (2) X-ray diffraction; (3) Electrophysiological and spectroscopic methods; (4) Single-particle methods, (5) Time-resolved electron scattering and X-ray diffraction techniques, and (6) Classical, quantum mechanical/molecular mechanical, and ab initio molecular dynamics simulations to study the essential protein machinery at the cell membrane.

## ■ Science of molecular engineering *(Designated in 2019)*

(Research trends) Materials science is an essential part of modern scientific endeavors for the advancement of humanity. Traditionally, the development of new materials has relied on serendipitous discoveries and “trial-and-error” optimization of properties. The latter is laborious, time-consuming, and expensive. In addition, the scope of materials science has immensely expanded in the last decades from metals, ceramics, and natural products to synthetic polymers, nanomaterials, and biomaterials. The properties and functions of these materials originate from the atomic- and molecular-level structures. Therefore, future demands of new materials to meet diverse and urgent societal needs require a new approach to the discovery and synthesis. Molecular engineering refers to the scientific approach to discover and synthesize new materials with desired properties and functions by cooperatively applying modern progress in theory, computation, physics, and chemistry. Radically different properties arise from crystals, of which the lattice topology is designed in such a way to exhibit electrical and thermal insulation only at the surface. Optical and electronic properties of organic semiconductors can be finely tuned to enhance the efficiency of energy harvesting and conversion. Biomaterials can also be designed and synthesized in such a way that the resulting materials intelligently deliver drugs and pharmaceutical cargo molecules to the target cells and organs. Metamaterials can be designed to exhibit unnatural phenomena, such as negative refractive indices, omnidirectional optical band gaps, and sound insulation. Ultrastrong materials can be designed by adopting minimal surfaces to distribute stresses in three dimensions. Non-equilibrium chemical systems that show response to external stimuli and adapt to the environment can be created. Polymers can be used as information storage media to permanently store large amounts of data without consuming energy. These prospects in materials science can only be realized by intelligently combining theory, calculation, experimental physics and chemistry, and biology.

(Necessity for IBS) IBS is an ideal venue for molecular engineering which requires interdisciplinary researches between fundamental theory, calculation, experimental chemistry and physics. Peer institutions recently launched departments dedicated to molecular engineering. Molecular engineering at IBS will help gain a highest-level scientific understanding of the structure-property relationship of materials and to establish scientific approaches to synthesize materials engineered to meet challenging requirements for future applications. This collaborative effort departs from the traditional approach based on discovery and optimization. Molecular engineering at IBS will contribute to solving urgent societal problems, such as energy, environment, and information technology.

(Key research contents) The proposed Center will focus on one or more of the following areas. (1) Nanoscaled/mesoscaled topological materials that exhibit unusual electrical/optical/sonic properties; (2) Intelligent biomaterials for drug delivery and cell division and proliferation; (3) New materials enabling high-density energy storage; (4) Polymers that can store and process information; (5) Non-equilibrium chemical systems that respond external changes by consuming energy; and (6) Ultra-strong and light materials based on minimal surfaces.

■ **Artificial photosynthesis** *(Designated in 2021)*

(Research trends) Artificial photosynthesis is an essential process in the harnessing of immense solar energy to induce the conversion of carbon dioxide to solar fuel and value-added chemicals. This technology can offer an environmentally-benign option for providing sustainable energy resources and solving global climate change caused by the increasing level of greenhouse gas. However, the slow reaction kinetics and unfavorable thermodynamics of CO2 reduction and water splitting are serious obstacles in establishing efficient photosynthesis technology. To achieve the artificial photosynthesis, diverse synthetic strategies based on semiconductor-based heterogeneous photocatalysts, bio-inspired homogeneous metal complexes, support-immobilized molecular catalysts, and biointerfaces composed of inorganic nanomaterials and biological systems have been exploited. One of the most crucial issues in artificial photosynthesis is the development of practically usable photocatalytically-active materials. Conventionally, trial-and-error-based Edisonian approaches have been widely used for developing artificial photosynthesis technology with a reference to the reported library of diverse photocatalytically-active materials and natural photosystems like PSI and PSII. Such non-systematic research strategies are not effective in accomplishing challenging research goals like artificial photosynthesis. Most of researches ever-reported failed to achieve sufficiently high overall efficiency for artificial photosynthesis. IBS intends to provide a solid platform to develop a new research paradigm for artificial photosynthesis from the collaborative works among experimentalists, theorists, and engineers. The combinative efforts from quantum theoretical calculation, materials synthesis, catalyst activity quantification, and device fabrication are indispensable for establishing practical artificial photosynthesis technology. For rational design of high-performance CO2 reduction/water splitting photocatalysts, fundamental understanding about the operation mechanism is of prime importance to establish crucial design factors for efficient photocatalyst systems. To construct effective photocatalytic cells for artificial photosynthesis, it is also necessary to exploit promising alternative oxidation reactions for replacing slow water oxidation reactions requiring four electron transfer.

(Necessity for IBS) The Center for Artificial Photosynthesis aims to develop practical technology of efficient artificial photosynthesis by accomplishing the fundamental understanding of underlying mechanism and design principles for catalyst synthesis and device fabrication. The establishment of commercially-available artificial photosynthesis technology requires collective efforts from a group of experts from various fields such as theoretical calculation, materials synthesis, materials characterization, and device fabrication. To achieve the proposed goal of artificial photosynthesis, stable research funding for long research periods is indispensable. This research subject is expected to make crucial contributions to solve two major challenges to human civilization, i.e., establishing renewable energy sources and mitigating global climate change, which would benefit from IBS-sponsorship.

(Key research contents) The researches in Center for Artificial Photosynthesis will cover the following topics:

(1) Theoretical design and mechanism proposal for artificial photosynthesis catalysts: Theoretical calculation-based rational designs of efficient photocatalysts with relevant electronic structures for CO2 reduction and water photosplitting. Elucidation of design factors for exploring optimized photocatalysts. Development of a new design paradigm for efficient artificial photosynthesis.

(2) Materials synthesis and activity validation: Rational and exploratory synthesis of efficient photocatalysts for artificial photosynthesis. Evaluation of photocatalytic performance for CO2 reduction and water photosplitting. Validation of proposed design rules for optimized photocatalysts. Elucidation of crucial factors in optimizing the overall efficiency of photocatalyst. Establishment of synthetic methodology to explore efficient photocatalyst for artificial photosynthesis. In-situ investigation for elucidating the operation mechanism of optimized photocatalysts.

(3) Photocatalytic cell design and fabrication: Exploration of alternative oxidation reactions to replace conventional water oxidation. Design and fabrication of efficient photocatalytic cells for artificial photosynthesis. Optimization of experimental factors to achieve high-efficiency CO2 reduction and water photosplitting.

■ **Immunomodulation** *(Designated in 2021)*

(Research trends) Modulation of immune response adopting the principles and tools of various science and engineering is one of the fast-growing research fields. Stimulating immune response selectively at the tumor sites demonstrates a great promise to enhance the therapeutic outcomes of cancer immunotherapy, where only limited patients respond efficiently by the currently available clinical products and methods. Also, the development of proper vaccine delivery systems to fight against infectious diseases becomes a critical issue in the pandemic era. On the other hand, suppressing or turning off the immune response (immune tolerance) has been tried as an effective strategy for treating autoimmune diseases as well as facilitating the tissue regeneration or tissue integration of medical devices.

(Necessity for IBS) Great progress in immunology led to clinically available immunotherapy. However, the effect is not general to all patients. Moreover, the level of understanding of the complex immune system is still not enough, especially with the exogenously administered immunomodulating materials. To pursue molecular, cellular, and materials-based approaches and to provide breakthroughs in the modulation of the immune system, multidisciplinary basic research combining expertise in immunology, (bio)materials, chemistry, nanotechnology, biotechnology, medicine, chemical engineering, and computer science is essential. Thus, this topic can be pursued with excellence by the IBS interdisciplinary center.

(Key research contents) Potential research topics in the proposed center include (but not limited to) (1) materials/nanosystems selectively stimulating immune response at the tumor to enhance the efficacy of cancer immunotherapy, (2) proper vaccine delivery systems boosting the immune system against newly emerging infectious diseases, (3) materials/nanosystems selectively reducing immune response for treating major autoimmune diseases (diabetes 1, arthritis, etc), (4) surface shielding or delivery system for providing immune tolerance of biological drugs, (5) immunology and engineering targeted for lymph node, (6) biomaterials and tools for T-cell engineering, (7) 3-D cellular structuring or organoids for in vitro/ex vivo modeling of the immune system, (8) biomaterials/systems for in situ manipulations of dendritic cells, (9) computational approaches for understanding and simulating the immune modulation.

■ **Ultralow-energy neuromorphic system** *(Designated in 2021)*

(Research trends) Bio-inspired neuromorphic computing has been suggested as promising technology for energy-efficient and high-performance computing system in the Big Data era. Neuromorphic computing aims to replicate the functions of neurons in cognition and to achieve the computing ability of the human brain. Current studies on artificial neural networks (ANN) for neuromorphic computing are mostly using traditional transistors with conventional computing architecture, i.e., the von Neumann architecture. However, such ANN leads to long-processing latency and high energy consumption, which is an obstacle to integrating neuromorphic devices up to 1012 (emulating neurons) or 1015 (emulating synapses), to mimic the human brain. To overcome the limits, several solutions for neuromorphic computing such as memristors (device level) and spiking neural networks (SNN, system level) have been suggested.

A memristor (memory + resistor) is a non-linear two-terminal device with its variable resistance depending on the history of the device operation. Multiple conductance states of memristors enable synaptic weights for neuromorphic computing. Memristors are arranged in crossbar arrays at each node, which resembles the structure of human cortex neural networks in that an analog functionality in the biological synaptic connection is inherent. Beyond the classical memristors, other emerging signal processing devices (based on spintronics, ferroelectricity, and ion transport) and materials (e.g., organic molecules and novel oxides) are considered promising for neuromorphic computing devices.

The SNN closely mimic the working principles of biological neural networks. In SNN, neurons communicate with each other through the sequence and timing of spikes, thereby enabling them to process time-series data. Compared to deep neural networks (DNN) or perceptron, the SNN consumes significantly lower energy for various neuromorphic computing including neural information processing, synaptic plasticity, and various learnings.

In accordance with recent development of novel materials and conceptual devices (e.g., 2D memristors and SNNs), dissipationless neuromorphic computing system could be realized by IBS.

(Necessity for IBS) The center for neuromorphic computing aims to conduct interdisciplinary studies to realize highly-integrated neuromorphic devices emulating the human brain. Conceiving new materials for reliable memristors and device architectures for large-scale neural networks is the key challenge for IBS. For that purpose, fundamental science and diverse engineering subjects should be extensively studied together in the center.

(Key research contents) The center seeks to realize highly-integrated neuromorphic devices for artificial intelligence.

(1) Materials synthesis: large-scale, reliable materials are required for memristors. Emerging oxides and 2D materials grown by sputtering or chemical vapor deposition (CVD) could be used with specific electrodes (e.g., Ag, graphene, etc).

(2) Device level: linear conductance response, multiple effective and reliable conductance states for synaptic devices, and low operation energy are required. A possible integration architecture (e.g., crossbar array) could be suggested and implemented with the device level study.

(3) Neural networks and computing level: diverse neuromorphic computing with feedforward or recurrent neural networks could be realized with the above materials and devices. Various activation functions for deep neural networks (multilayer perceptron) and convolution neural networks could be run with a low operation energy.