# Details of Designated Research Areas

## ① Mathematics / Computer science

### ■ Scientific computing *(Designated in 2012, revised in 2019)*

This area has developed into a key strategic field due to rises in the scope of its industrial application. Undoubtedly, it addresses core questions related to the modeling of situations arising in various areas of science and engineering, including mechanics, physics, and chemistry. The subject requires familiarity and proficiency with advanced mathematical tools and concepts, with possible applications to Computer Science, Engineering (in particular, Fluid Mechanics), Biology or Genomics, etc. without being entirely specialized in any of these areas.

- Scientific Computing: Mathematical theories involved in computer science and applications
- Numerical Structure: Developing numerical methods to solve mathematical problems
- Quantum Computing: Mathematical theories of quantum computation
- Including but not limited to the above areas of study

### ■ 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

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

(Research trends) The development of new imaging modalities in areas such as biomedical, biological, molecular structure, nanostructure, and field imaging is helping to overcome current imprecisions and limitations, thus leading to clearer visualizations of various physical phenomena. New areas of mathematics in imaging are emerging and overcoming limitations in existing mathematical frameworks. Besides, recent advances in machine learning are expanding our ability to analyse images through training data. Collaborative research among diverse fields of science and technology related to imaging is therefore very desirable.

(Necessity for IBS) The Center of Mathematics of Imaging aims to improve existing imaging modalities and develop new ones by employing a deep understanding of the mathematical structures in existing imaging techniques. Imaging science is multidisciplinary in nature, involving mathematics, biophysics, engineering, and medicine. To make discoveries and achieve research breakthroughs in imaging science, the Center should be composed of multiple principal investigators with distinct, but complementary, expertise. Given the resulting continuous close cooperation among these specialists, the Center will perform cutting-edge multidisciplinary research across the wide field of imaging.

(Key research contents) The Center's research covers four main areas: 1) Mathematical modeling and analysis of various imaging techniques in biomedical and biological imaging, imaging of nano-structures, etc.; 2) Analysis of measurement data, new algorithms for image reconstruction, and numerical simulations; 3) Machine learning for image analysis and developing mathematical theories for feature representation learning;

and 4) Interdisciplinary research in the fields of mathematics, physics, biology, and medical sciences.

Given that each existing imaging modality has limited capabilities, the development of mathematical models that provide additional information from images requires fusing the knowledge and techniques of various fields. To develop new comprehensive imaging techniques that offer significant practical improvements, it is necessary to understand fully the physical phenomena underpinning data-acquisition systems as well as the implementation details of algorithms. Deep image analysis will rely on machine learning, and highly sought-after mathematical theories will contribute to understand how feature representation is created by deep learning.

## ■ Data science and analytics

### • Data Science *(Designated in 2017, revised in 2019)*

(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.

(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 group 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 research group 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 Group 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.

- **Mathematics of deep learning** *(Designated in 2019)*

(Research trends) The mechanism of human learning is undergoing a paradigm shift due to a remarkable and rapid development of deep learning skills. The latter have expanded our ability using sophisticated nonlinear regressions through data training. They are expected to overcome limitations of existing mathematical methods in dealing with various ill-posed problems, such as image reconstruction with insufficient data, e.g., undersampled magnetic resonance imaging and sparse view computerized tomography. It is strongly expected that deep learning methodologies will improve their performance as training data and experience accumulated over time.

(Necessity for IBS) Although deep learning has accomplished great successes in various areas including science and medicine, there is a tremendous lack of a rigorous mathematical foundation which 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 group include 1) Mathematical foundation for explaining and interpreting deep learning models; 2) Data science for deep learning; 3) Manifold learning for disentangled feature representation; and 4) Deep learning applications to automated image analysis, pattern recognition, and medical sciences.

## ② Physics

### 1) Theoretical physics

#### ■ Theoretical fundamental physics

• **Particle & nuclear theory** *(Designated in 2012)*

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

• **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

- **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 Center 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 computer** *(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 Computers 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)*

The goal of this area is to understand, within the framework of physics, macroscopic phenomena emerging in condensed-matter systems, biological systems, information and communication systems, as well as in social and economic systems. Studying such complex systems help elucidate phenomena which would otherwise remain unpredictable using a traditional reductionist approach.

· Studying nonequilibrium statistical physics in open systems and disordered systems: nonequilibrium fluctuation theorem; phase transitions and critical phenomena; dynamical scaling behaviors; transport and diffusion in disordered systems

· Studying the science of complex networks: theoretical studies of structures and dynamics of complex networks; application of the theory of complex networks

· Studying the dynamics of nonlinear/nonequilibrium systems and pattern formation

· Dynamics and structures of soft matters such as polymers, gels, liquid crystals, microemulsions, foams, colloids, granular materials, etc.

· Including but not limited to the above areas of study

## • Biological physics *(Designated in 2012)*

The goal of this area is to illuminate the physical principles of living phenomena and to investigate the microscopic phenomena of life and complex systems.

· Understanding the physics in the functions of biomolecules

· Systematic understanding of the molecular-level operation principles of biomolecules and complexes

· Understanding the brain using computational methods

· Discovery of new drug candidates and development of disease diagnostic methods using bio-network analysis

· Theoretical studies of biological membranes, proteins, DNA, etc.

· Including but not limited to the above areas of study

## • 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<br><br>· 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)*

(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 include LIGO and Virgo for GW, 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 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.

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

1) Gravitational waves. Development of a new type of GW detector, which is not covered by LIGO and Virgo. 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. A large neutrino detector with the necessary energy resolution to detect neutrinos from cosmic explosions accompanied by GW and/or EM 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.

## ■ Ultrafast X-ray and optical science *(Designated in 2017)*

(Research trends) Understanding the interplay between various subatomic components, such as electrons, spins, and microstructures, is essential in materials studies. Recently emerging ultrafast science aims to obtain a fundamental insight into an extensive range of materials properties, by probing the ultrafast processes involving electrons, spins, and microstructures in atomic- or nanometer-scale. Currently, ultrafast pump-probe techniques are available with near-infrared, terahertz, and optical lasers, and newly developed X-ray free-electron lasers (XFELs). These techniques can be applied to study very fast charge, spin, and structural dynamics, and their coupling in complex materials systems. Outcomes from these studies can lead to a better understanding of key properties of complex materials systems, and possibly allow the discovery of novel phenomena and new functional materials system for the development of next-generation devices.

(Necessity for IBS) The Center for Ultrafast Science aims to understand structural dynamics of a wide range of materials using ultrafast X-ray and optical techniques. A cutting-edge light source and various characterization techniques consolidated by the Center will open new opportunities to investigate and to control material properties on a femtosecond time scale with subnanometer spatial resolution. The close interactions with other IBS groups will generate a synergistic effect to produce novel ideas and innovative research tools. Moreover, the research groups in the Center will be independent yet closely linked to each other, valuing the spontaneous collaboration and clash of ideas. The Center can be directed by co-principal investigators, e.g. light source scientist and light-matter interaction expert, operating mutually complementary research units. The studies conducted by the combined efforts and knowledge provided by the Center will provide a fundamental understanding of unresolved problems, which will direct the tailoring of materials properties in various complex materials systems.

(Key research contents) The Center's research is composed of 1) XFEL science and ultrafast optics; 2) Dynamics of strongly correlated systems; 3) Magnetism and ultrafast devices; 4) Ultrafast dynamics in liquid systems. Development of high resolution and ultrafast instruments such as ultrafast electron diffractometer, spectroscopy, and microscopy will provide opportunities to study ultrafast dynamics of electrons, spins, and structures in a short time domain, and to understand the fundamental properties of complex material systems. In addition, ultrafast coherent X-ray imaging and scattering, femtosecond pump-probe, X-ray nanoscale crystallography, ultrafast optical excitation and detection, nonlinear optics in EUV and X-ray regimes will provide optimal ultrafast instruments for problem-driven studies.

Using the above ultrafast techniques, dynamics of strongly correlated systems will be investigated to understand pathways for phase transition of topological insulators and 2D materials, lattice dynamics in superconductors, Mott insulators, Weyl semimetals, and chiral systems.

Another research line will deal with fast spin dynamics, to fundamentally understand magnetism, such as dynamics of magnetic order and domains, excited-states dynamics of Skyrmion in nanoscale, magnetic insulator, and to develop ultrafast spin-based devices.

Electrolyte solutions, solvation and chemical reactions, heat propagation, homogeneous nucleation, and biphasic separation all involve ultrafast phenomena in liquid systems. Therefore, understanding of ultrafast dynamics in microscale is essential not only for a deeper understanding of liquid properties but also for its enormous practical potential. This interesting subject of liquid systems has been not much explored yet and awaits systematic investigations utilizing state-of-the-art tool with temporal and spatial resolutions.

Based on the understanding of the relationships between electronic, magnetic and structural order with ultrafast science, the Center should provide opportunities for novel findings and applications in complex materials systems.

## ■ 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 2019)*

(Research trends) Quantum technologies, including cold atoms and quantum information processing and communication, have the potential to revolutionize many fields of basic science and technology. This research area has developed from atomic, molecular and optical (AMO) physics. It exploits a fundamentally new model of computation and communication, 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 quantum information technology in the US, EU, UK, Canada, China, and Japan. The research related to quantum technologies requires extensive fundamental studies and approaches from diverse fields of physics, including quantum optics, atomic/molecular physics, and semiconductor/superconductor physics.

(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 related to quantum technologies. 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 (SPDC), 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.

■ **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

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

### ■ Nuclear Physics *(Designated in 2015)*

Nuclear physics has been one of the key fields in physics, together with particle physics and astrophysics. Nuclear physics in rare isotope (RI) pursues the investigation of the fundamental interactions of nuclei and their constituents, as well as structures of stable and unstable nuclei. Going deeply into the uncharted regime of exotic nuclei, far from the stability regime, can probe the structure of nuclear forces, such as tensor forces and many-body forces. Experimental nuclear physics with RI beams, in close collaboration with theoretical studies, is critical for the success of the RI accelerator in Korea.

- Structure: Structures of radioactive isotopes and stable isotopes, new rare isotopes, drip lines, new magic numbers, tensor forces
- Astrophysics: Origin of the elements, nuclear reactions in the r-process, evolution of stars, elemental abundance ratios in stars, structure of neutron stars
- Reaction: Equation of state for asymmetric matter, 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 for dense matter, reaction mechanisms
- Including but not limited to the above areas of study

### ■ Applied RI sciences

#### · Condensed matter physics *(Designated in 2015)*

The convergence of condensed matter physics and nuclear physics provides new powerful tools to study materials. The application of extremely sensitive methods and devices developed by nuclear physicists has been shown to be advantageous for investigating the electromagnetic properties of materials. Among them are muon Spin Rotation, Relaxation or Resonance (μSR) and beta-radiation-detected Nuclear Magnetic Resonance (β-NMR), which are considered to be the main facilities for material science research at the rare isotope (RI) accelerator in Korea.

This area aims to study the nature of materials by using μSR or β-NMR. A plan for training experts through fundamental researches or applications in the broad area of condensed matter physics should be established for the success of the RI accelerator in Korea.

· **Radiation biology / Oncology and medical physics** *(Designated in 2015)*

This area deals with the effects of heavy ion beams, including RI beams, on organisms and tumors. It is based on principles, methodology, and practical dosimetry of heavy ion irradiation. Research topics include, among others, biological responses and mechanisms correlated to the exposure of heavy ion beams, relative biological effectiveness of heavy ion beams, significance of heavy ions in cancer treatment, calculation and verification of heavy ion absorbed dose, precisely tumor-conformal heavy ion irradiation, as well as in-beam imaging of heavy ion irradiation. The studies of radiobiology and medical physics should be co-operative and integrated. The outcomes achieved in this area will be useful to understand the responses of living things when exposed to heavy ion beams and to treat intractable cancers.

· **Nuclear energy / Nuclear data** *(Designated in 2015)*

Fast nuclear reactor systems are proposed worldwide as possible future sustainable nuclear energy solutions to solve the problem of spent nuclear fuels. In order to realize such systems, development of an experimental facility for a subcritical fast reactor system and comprehensive studies for accurate data of relevant nuclear reactions are needed.

As part of RAON application, this research area aims to develop an experimental facility for a fast reactor system, optimized for integral neutronics experiments and precise measurements of the required reaction channels. Experimental measurements and theoretical investigations will be performed to obtain reliable nuclear cross-sections and decay data of radioactive isotopes, which are still largely unknown, to improve the accuracies of the existing nuclear data with covariances, and to enhance the safety and integrity of fast reactor systems.

· **Atomic and molecular physics** *(Designated in 2015)*

This area is designated to study fundamental properties, such as masses, lifetimes, hyperfine structures and isotope shifts of atoms, by using heavy ion beams, including RI beams. The rapid advance in the field of heavy ion accelerators, as well as experimental techniques of electron beam ion trap (EBIT), laser cooling, and collinear laser spectroscopy makes it possible to investigate atomic structures and properties of stable or radioactive isotopes. In addition, collisional and radioactive processes can be investigated with RI beams. Information on the charged states and nuclear charge distribution of an atom or an isotope as well as its level structures are crucial in the analysis of collisional and radiative interactions. Such analysis requires relativistic theoretical treatment as well. Precision electric dipole moment (EDM) measurements of rare isotopes can reveal the influence of nuclear structure on atomic properties, which will allow us to test physics beyond the Standard Model.

· **Other RI sciences** *(Designated in 2015)*

Other sciences using the RI accelerator facility that are not covered above should be included.

## 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)*

(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 owing to the manifestations of various irreversible age-related diseases, which are preventing the increase in healthy life expectancy, thus burdening healthcare costs worldwide. The emerging discoveries and challenges related to aging processes have prompted scientific communities and global pharmaceutical companies to start regarding aging processes as diseases, which should be intervened upon and even reversed in the future. Scientists are now searching for fundamental mechanisms for the aging of organisms utilizing various models including humans, and are employing comprehensive modern scientific knowledge and techniques such as 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 aging process.

(Necessity for IBS) Research on aging has been pursued vigorously 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 via animal model systems, including 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 national level. The IBS Center for Aging Biology needs to become the hub that connects basic scientists and clinicians aiming to understand the fundamental processes of age-related phenomena, bringing novel ideas to intervene in and retard aging, and ultimately providing an increase in healthy life expectancy for the future generation. The areas to be covered will involve a combination of studies on genetics, genomics, immune systems, metabolic syndrome, regenerative medicine including stem cells, etc.

(Key research contents) The focus of this research is to understand human aging as a disease that progresses and can be cured. Therefore, the research will cover molecular, cellular, genetic, physiological, and clinical biology, focusing on human aging and age-related pathologies. 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 employing animal model systems including Caenorhabditis elegans, fruit flies, mice, zebra fish, 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 metabolic syndromes that affect life span, the molecular and genetic aspects of caloric restriction, oxidative stress, mitochondrial function, molecular hormone responses, microbiotal changes, muscle/skeletal deterioration, etc. need to be pursued. In addition, studies on age-related deterioration of the adaptive and innate immune system, inflammation, autoimmune diseases, etc., using model systems 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 2019)*

(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 three key questions in mammalian developmental biology are still unanswered. Revealing the identity of a cell and its time-dependent regulation (chrono-developmental biology) are fundamental inquiries of biological sciences. All cells of an organism have identical copies of genetic information, and it is their different developmental program that leads to their distinctive developmental fates. Developmental fate determination is affected by transcription control in space and time, differentiation, epigenetic regulation, chromosome dynamics, etc. Developmental fate determination involves transcription control in space and time, differentiation, epigenetic regulation, chromosome dynamics, etc. Many diseases of somatic cells, particularly cancer, are a mere recapitulation of a wrong development. Therefore, understanding the programming of this developmental process is key to understanding diseases as well. 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 unresolved.

(Necessity for IBS) One should be asking such bold questions as "What is the molecular basis of differentiation in genetic/epigenetic control?" at the IBS Center for Developmental Cell Biology (DCB).

1) Unveiling transcriptional and epigenetic control of stem cell maintenance; 2) Stem cell differentiation; 3) Symmetric and asymmetric division of cells in development; 4) Dynamics in cellular organelle; 5) Understanding development in time and space; and 6) Development of novel imaging techniques for live embryos.

(Key research contents)

• Genetic programming and reprogramming of stem cells
How genes control the growth and development of an organism throughout its life-cycle should be studied. Furthermore, elucidating the stemness is also an important subject to understand how cells constitute tissues, and how cells grow and differentiate. Using genetically modified animal

models and adopting novel stem cell technologies, including iPS, 3D organoid culture, or any novel culture techniques in stem cell studies, the Center will provide opportunities for: understanding how genetic programming and reprogramming turns on cell differentiation, novel findings in the maintenance of stemness, and applications in treating human diseases.

• Dynamics of cellular membranes and organelles
Owing to the developed omics and imaging technologies, physiological functions of various cellular organelles have been revised. For example, plasma membranes cannot be explained by a classical fluid mosaic model and mitochondria are not simple energy factories. In addition, cellular organelles are interconnected, regulating cell functions. Reexamining cellular organelles (plasma membrane, mitochondria, chloroplast, endoplasmic reticulum, Golgi complex, lysosomes, endosomes, caveolae, lipid rafts, cytoskeleton, extracellular matrix, extracellular vesicles, tunneling nanotubes, cilia, etc.) might give us fundamental knowledge about all living organisms.

• Developing novel imaging techniques in live embryos
Owing to developmental biology studies, such new technologies as in vitro fertilization and stem cell therapy have been developed. Similarly, progress in super-resolution, live-imaging techniques in living embryos will open a new horizon in the field. It will provide new therapeutic clues to dysfunctional developmental disorders in humans.

• Chrono-developmental biology
All organisms are under the influence of 'time'. Accordingly, sensing and operating systems for the 'circadian rhythm' are found in most organisms on Earth from bacteria to human beings. 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 must be a 'master clock' able to communicate with all the cells that controls the course of complicated events during development. The recent advent of stem cell biology and regenerative medicine prompts the fundamental importance of developmental biology. Synchronization of the development of each part of the body is extremely important for proper development, but it is one of the least understood phenomena in biology as well. Therefore, developmental chronobiology 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 2019)*

(Research trends) As technologies and analytical platforms in individual omics analyses, such as genomics and proteomics, have been established, integrated omics analysis has emerged for a holistic understanding of cellular events in disease-related cells, tissues, or organs. Several representative consortium projects, such as The Cancer Genome Atlas (TCGA), Human Microbiome Project (HMP), Brain Initiative, Precision Medicine Initiative (PMI), and Cancer Moonshot have employed diverse integrated omics analyses involving different combinations of global analyses. Cardinal pillars in the integrated omics analysis are 1) global analyses to generate diverse types of comprehensive data in disease-relevant cells, tissues, or organs, including sample preparation methods and developments of analytical instruments and reagents; and 2) computational methodologies for integration of different types of biological information produced from individual omics analyses to generate hypotheses about fundamental principles of human diseases. Despite recent advances in omics technologies and data analyses, there have been still significant needs for new global analysis technologies and data integration methodologies to generate more relevant and reliable hypotheses about fundamental principles of human diseases, involving dynamically changing multiscale cellular processes. This research is designed to address challenging biological questions that remain to be answered by developing or applying creative~~ly~~ integrated omics analyses.

(Necessity for IBS) Owing to their 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.) have been standardized. However, compared with individual omics, integrated omics requires new technologies and methodologies based on a combined understanding of: genomics, proteomics, imaging, informatics, phenomics, biochemistry, in vivo and clinical models, technology development, etc. Examples of the technology development include single-cell level proteomics for intracellular signaling networks, interactomics for decoding dynamic evolution of interaction networks, etc. Accordingly, no single researcher can handle this research in the full spectrum, and tight collaboration among researchers with diverse expertise is essential for the success of the perspective Center for Integrated Omics.

(Key research contents) Integrated omics itself may not be sufficient to justify the need for a new IBS Center. Thus, a creative biological question for challenging problems that can lead to innovative and transforming outputs, but cannot be answered effectively without integrated omics analysis should be first defined. A detailed integrated omics approach should be then designed to effectively answer such biological question. Then, new global assay technologies will be developed or existing global assay technologies will be applied, and the methodology to integrate multiple types of global data will have to be clarified. These activities would also have to involve tight collaborations with engineers, bioinformaticians, or clinicians. Finally, the potential impacts of the research outputs on advances or innovation of biology or medicine should be clearly addressed.

## ■ **Immunobiology** *(Designated in 2019)*

(Research trends) Identifying various types of immune cells and understanding their functions and regulation have been fundamental issues in the immunology field. While our understanding of immune cell development and responses in lymphoid organs has been significantly advanced over the last few decades, those in non-lymphoid organs have only begun to be understood. New types of immune cells exhibiting mixed features of multiple conventional immune cells, such as CD4 T cells that simultaneously express a combination of Th1, Th2, and Th17 cytokines, have been identified in inflamed non-lymphoid organs. However, their origins and developmental processes, as well as functions, remain poorly understood. On the other hand, in the gut, there is a considerably important and intimate cross-talk between the microbiota and immune system, affecting immune cell differentiation and functions to maintain our body immune homeostasis. These types of immune reactions that occur in non-lymphoid tissues have received a lot of attention from immunologists to comprehensively understand our complex immune system and pathogenic mechanisms underlying related immune disorders. Therefore, it is important to unravel how tissue environments specifically affect immunity and the meaning of these immune responses at organism levels.

(Necessity for IBS) Compared to other research areas, immunological researches are heavily dependent on genetically engineered mouse models. Since many mouse models useful for the immunological researches are commercially available, securing these mice in a research institute is one of the key elements that contribute to competitiveness in the immunology field. Immunological studies also necessitate cutting-edge technologies including fluorescence-activated cell sorting (FACS), single-cell RNA sequencing, and in vivo imaging systems. Since the maintenance of these research facilities requires a large amount of stable funding, it is very difficult for an individual lab to undertake competitive science in the immunology field. Therefore, a research Center equipped with various core facilities for immunological studies is urgently required to pursue world-leading science. Moreover, this perspective Center would provide excellent research platforms to immunologists in Korea.

(Key research contents) The Center for Immunobiology will primarily focus on immune responses beyond classical immunity. Research topics in this subject may include 1) Identification and characterization of novel types of immune cells; 2) Relevance of these immune cells to the pathogenesis of immune disorders in humans; 3) Interaction between tissue environment and immune cells; 4) Immunometabolism governing a variety of immune cell differentiation; 5) Role of microbiota in immune homeostasis, etc. Other fundamental researches that could potentially make a breakthrough in the immunology field will also be pursued in this Center.

■ **Molecular biology & chemical genetics** *(Designated in 2017, revised in 2019)*

(Background) Studies on the molecular machinery that govern cell growth, differentiation, disease, and death have been heavily investigated, yet underlying molecular basis of many life-threatening diseases remain to be understood. Recent progress in gene editing, high-resolution imaging, chemistry applied to biology, and omics technologies in model organisms provide an unprecedented opportunity to tackle the question of life, growth, disease, and death. The adoption of CRISPR in gene editing has revolutionized the manipulation of genes in any organism, contributing to the discovery of molecular pathways in disease, but its use in humans is still in debate for ethical reasons. Applying chemicals to block, trigger, and modulate molecular pathways can compensate for the resistance of CRISPR in humans and live animals and represent a powerful tool for understanding the basis of disease. Moreover, one of the chemical genetics' strength is that it can be directly applied to clinics.

(Necessity for IBS) The Molecular Biology and Chemical Genetics (MBCG) aims to unveil cellular pathways in understanding the basis of human diseases using genetics and molecular biology in various model organisms (mouse, Drosophila, C. elegans, yeast, etc.). The Center will be composed of groups using different disciplines in molecular biology and chemical genetics, but with the common aim to understand the basis of unsolved disease. The close interactions between the groups using distinct research systems will generate a synergistic melting pot that encourages novel ideas and innovative research tools. The Center can be the liaison of other IBS Centers and domestic institutes, as this Center will provide molecular, chemical, and genetic tools and techniques with appropriate model organisms nationwide. Such interdisciplinary research Center will constitute a collaborative cluster that promises the emergence of novel techniques and fields. This is what IBS is for.

(Key research contents)

- Chemical genetics: Controlling biological processes and manipulating selective pathways with chemicals can lead us to understand the basis of human diseases, while providing promising platforms for drug development. Combined with gene editing technology, cutting-edge research in chemical genetics will serve as a powerhouse for a fundamental understanding of diseases and direct application to molecular, pathway-directed, precision medicine. The development of model organisms is expected.
- Molecular omics approaches in human and model organisms: Genomics, proteomics, and network biology in man and genetically engineered model organisms will reveal the regulatory modules and signal transduction pathways that control life, disease, and death. The molecular omics technology, when combined with rigorous molecular cell biology in genetically modified organisms, will provide opportunities or developing new targets and biomarkers of human diseases.
- Epigenetics in human and model organisms: Epigenetic change can be influenced by external or environmental factors including developmental stages and disease states. Although most epigenetic changes occur within the course of one individual organisms' lifetime, some epigenetic changes can be inherited to the next generations. Using genetic and genomic approaches, the Center address epigenetic contributions in the development of various human diseases.
- Biophysics and biochemistry for biomedical research: High-resolution imaging, single-molecule FRET, TIRF, live-cell imaging, high-resolution cryo-EM, etc. made revolutionary changes in biomedical research. The Center should aim for continuous development of novel techniques. Often, these developments come from close collaboration with physical chemists and physicists. Co-PIs, who are trained in chemistry, physics, or even engineering, may work well together with geneticists, stem cell biologists, and molecular biologists, when they share a common interest in understanding the basis of human disease.

■ **Emerging infectious diseases** *(Designated in 2017)*

(Research trends) Emerging infectious diseases (EIDs) are those whose incidence has increased in the last 20 years. EIDs are caused by newly emerging or evolved pathogens (e.g. SARS and avian influenza), re-emerging pathogens (e.g. Ebola, malaria, and tuberculosis), or antibiotic-resistant pathogens (e.g. superbugs). As we have experienced from the recent case of MERS spread, the devastating impact of infectious diseases, especially those which propagate through the air, is not limited to an individual health problem, but challenges various socio-economic aspects of our country. Nationally-trusted and globally-competitive science is in need to unravel the mechanism of the infectious diseases that have the biggest impact on Korean society, and to find ways to keep these diseases under control. The rapidly evolving infectious agents, which include viruses, bacteria, and fungi, require comprehensive front-edge approaches to diagnosis, prevention, and cure. The rapid spread of antibiotic-resistant pathogens is another challenge to overcome, especially in Korea.

(Necessity for IBS) Research on infectious agents requires intensive collaboration among virologists, bacteriologists, chemists, immunologists, epidemiologists, and medical doctors. It also needs a core facility to handle and confine infectious agents. Despite the urgency and importance of this research in Korea, only a limited number of individual labs are carrying out quality research of international competence. The Center will create a synergistic environment, recruiting both leading and promising researchers to understand air-borne EIDs. Trans-disciplinary efforts will reveal pathogenicity mechanisms of the infectious agents and the response of animal hosts, getting closer to understand and control EIDs.

(Key research contents) The Center's research will focus on 1) Viral respiratory infections; 2) Pneumonia; 3) Tuberculosis; and 4) Antibiotics-resistant infections. Viral respiratory infections (VRIs) are illnesses caused by a variety of viruses that affect the upper respiratory tract. The etiological viruses are mostly RNA viruses such as the influenza viruses and the coronaviruses. They can evade the therapeutic measures and also cause more and more severe illness, due to their capability of very rapid adaptation primarily based on the high mutation rate of their RNA replication system. Comprehensive analyses of their genomic evolution and pathogenic trait alteration, as well as host cell response are in need to elucidate the mechanism of pathogenicity and rapid evolution. Respiratory infections eventually lead to a complicated lung disease called pneumonia. In-depth scientific studies on pneumonia-causing pathogens and host immune responses are needed to develop efficient diagnostics and vaccines. Another research area is epidemic antibiotics-resistant infections, caused by numerous "superbacteria" and multidrug- and pandrug-resistant bacteria. Focused multi-disciplinary research on the molecular mechanisms of diverse antibiotics-resistance pathways of the major resistant bacteria (sometimes referred to as "ESKAPE pathogens") and mechanism of antibiotic action is needed to unveil hidden keys to control drug-resistant bacteria, such as drug-resistant TB (tubercle bacillus).

## ■ Phytobiology *(Designated in 2019)*

(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 question in fundamental 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. At the subcellular and molecular level, they study how genome-encoded molecular information (proteins and DNAs/RNAs) regulates the biological processes in response to environmental changes. At the cellular level, they study how cells' interactions lead to complex responses during development. They also study how these biological processes interact and are integrated.

(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. In order to do competitive science in phytology field, the study requires a coordinated effort by a broad spectrum of expertise, including plant molecular genetics, plant developmental biology, plant tissue culture, genomics, phenomics, metabolic analysis, genome editing technology, etc., and related facilities as well. Only IBS can manage such coordinated collaborative basic research, and the Center will provide excellent research platforms for plant scientists in Korea.

(Key research contents)

- Temperature signaling network of plants
  Research on temperature biology examines the fundamental question of how plants perceive and respond to changes in ambient, non-stress temperatures. 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
  Light signaling governs every facet of plant development from seed germination to seedling development, from vegetative growth to flower development. However, the mechanisms by which photoreceptor systems regulate the intricacies of plant development are still unclear. 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 molecular genetics and physics will provide new tools customized to study plant responses to light.

- Hormone signaling network of plants
  The form and function of plants are mainly determined by efficient communications among cells and cross-talks with environmental stimuli. 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. The information obtained from this research area will address the fundamental question on how plants control de-differentiation processes, bringing us closer to the understanding of plants' life.

- Regulation of plant vegetative development
  Plants monitor and integrate environmental cues to optimize their survival and reproduction, and carefully modulate their vegetative growth. Thus, 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. The knowledge obtained from this area will be

useful to understand how plants decide their cells' fates and to explain the evolutionary trajectory that occurred during land plant evolution.

- Regulation of plant reproductive development
  This research studies how plants regulate the series of orderly changes in their reproductive development, including flowering time, floral patterning, fertilization, 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. This area is especially important because 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.

- 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.

## ■ Systems neuroscience *(Designated in 2017)*

(Research trends) The brain contains trillions of interconnected cells and possibly more than 1,000 types of neurons. Many world-class research centers (e.g., the Allen Institute for Brain Science and Janelia Research Campus) are investigating specific characteristics of each neuronal cell type~~s~~, including molecular composition, morphology, synapse profiles, and firing patterns. Blueprints underlying brain development and functions are encoded in the genome, and rapid technical advances have facilitated multi-omics data analysis of brain cells or tissues for large patient cohorts. For instance, Iceland has recently compared whole genome sequence data of 1,500 Alzheimer patients with those of 150,000 negative controls (~half of the whole population), which would provide unprecedented information and understanding of this neurodegenerative disease. The whole transcriptomic and proteomic data of neurons can also be obtained at the single-cell level, and analyzed 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 electro-physical 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.

(Necessity for IBS) 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, consciousness, 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 (3D morphology, neurite branching, and synapse distribution), functional profiling of neurons (intrinsic neuronal excitability and firing), and neuronal circuit mapping and control. For big data analysis of the brain in health and disease, future IBS centers would have to systematically collect and analyze global data on genomic, transcriptomic, proteomic, excitation, and firing profiles of specific neuronal cell types. The centers also develop and use advanced tools/platforms for the big 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

### ■ Anthropogenic climate forcing and biogeochemical cycles *(Designated in 2012)*

- Enhancing knowledge of sources, sinks, and their geographic patterns in the cycling of biogeochemical greenhouse gases (GHGs); and understanding spatial and temporal multi-scale factors regulating these multidisciplinary processes
- Supporting advances across a robust mix of atmospheric, oceanic, land- and space-based observing systems and data assimilation for the monitoring of recent climactic data relevant to chemical/radiative species
- Refining the industrial processes and emission sources of industrial gases with high Global Warming Potential (GWP) to understand environmental problems related to the large economies of East Asia
- Including but not limited to the above areas of study

### ■ Responses of marine ecosystem *(Designated in 2012)*

- Understanding physical environmental processes and their changes in terms of their effect upon the ocean ecosystem structure and biodiversity to diagnose the current status of the oceanic environments
- Investigating the impact of the anthropogenic forcing on oceanic ecosystem and biodiversity through global scale and long-term monitoring to preserve and protect both the oceanic environment and its biological resources, and thus allow for the sustainable use of the oceans
- Integrating changes in biological production of functional groups and the functioning of marine food webs
- Studying the past through close examination of various paleo-samples in oceans to project the future
- Including but not limited to the above areas of study

### ■ **Coastal zones including extreme events** *(Designated in 2012)*

- Assessing the extreme climactic events induced by changes in the climate, and also investigating natural catastrophic events (e.g., earthquake, tsunami and volcanic eruption) in association with the geological processes within the Earth's interior
- Studying the current state of, and any changes in seawater temperature, sea level, typhoon activity, carbon cycling, water cycle and dissolved elements transport, and ecosystem as a whole in coastal environments
- Investigating the influence of a rise in sea levels on the characteristics of seawater-freshwater interaction, and the physicochemical and thermal properties of groundwater and coastal water
- Including but not limited to the above areas of study

### ■ **Integrated impact assessment** *(Designated in 2012)*

- Delivering integrated multidisciplinary assessments of the overall effects and impacts on both local and global scales
- Integrating the development of appropriate models covering a wide range of time and space scales and multidisciplinary scientific data in order to maximize the utility and societal benefits of the assessment, through economic and social data
- Developing appropriate predictive models to deliver suitable advice for the socio-economic and policy impacts of change
- 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.

■ **Next-generation catalysts** *(Designated in 2019)*

(Research trends) Conventionally, semi-empirical approaches have been used for developing catalysts with the aid of theory. IBS seeks to host a Center for Next-Generation Catalysts toward creating a new paradigm for designing optimal catalysts from quantum theoretical principles, followed by experimental synthesis and validation. In particular, the sought-after catalysts should address critical societal issues related to sustainable energy and environment. A photo-catalyst for water splitting at ambient temperature is a prime example, as it will enable the harnessing of unlimited solar energy as is done by plants in photosynthesis. Several semiconductor-based artificial photosynthetic systems exist; however, the overall efficiency is low and needs a drastic improvement to be practical. The challenge is to create a highly efficient catalytic system to make molecular hydrogen economically accessible as a clean fuel. Hydrogen thus produced may also be used to reduce $CO_2$ to methane or other value-added species using another catalytic system. In designing both catalysts, understanding and controlling the electron dynamics involved should be critical. Current-generation approaches to catalyst developments are rather limited in scope and are extremely time-consuming, because the range of combinations in design parameters is practically limitless. Quantum theoretical and computational science have advanced remarkably in recent years so that new designs of next-generation catalysts for water splitting and $CO_2$ reduction can be attempted, potentially with the aid of artificial intelligence (AI) techniques. The design rules should take thermodynamic and kinetic considerations into account. The candidate systems must be synthesized and tested for continued improvements in efficiency.

(Necessity for IBS) IBS aims to be a world leader in basic research by focusing efforts to selected scientific goals. Securing sustainable energy sources and preserving the planet are the two key challenges that should be met for continuing human civilization. IBS needs to focus on high risk, high return projects which could have impacts on critical scientific and societal issues.

(Key research contents) The Center should strive to achieve:

(1) Theoretical designs of optimal catalysts both for generating hydrogen from water and for reducing $CO_2$ to hydrogen-rich fuel. The design should be based on sound quantum theoretical considerations and be approached with thorough computations. Elucidating catalytic systems often involve non-trivial electronic structures, and developing new approaches for tackling such systems will be highly desirable. Machine learning approaches can be utilized to facilitate optimal designs. Efficient tactics for accumulating crucial data should be embedded. Optimizing catalysts will inevitably involve searching through diverse molecular modifications, and strategies should be constructed for exploring and expanding such diversity.

(2) Experimental demonstrations on highly efficient optimized catalysts. Experimental data from the candidate heterogeneous catalysts could guide further theoretical developments. Optimized systems should be realized by syntheses and be demonstrated toward their catalytic efficiencies. Imaging techniques should be employed to visualize and verify the catalytic processes with high spacial and temporal resolutions, and to help understand the catalytic mechanisms.

■ **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.