World Premier International Research Center Initiative (WPI) Executive Summary (For Extension application screening)

Host Institution	Tohoku University	Host Institution Head	Susumu Satomi
Research Center	Advanced Institute for Materials Research (AIMR)	Center Director	Motoko Kotani

A. Progress Report of the WPI Center

I. Summary

AIMR was established to create new materials with innovative functions, construct devices based on new fundamental paradigms, and contribute to society by building a foundation for safe and enriched livelihoods. These are conducted by our world-leading organization for interdisciplinary research through an innovative method of atomic and molecular control departing from traditional approaches. In the FY2011 Interim Evaluation, AIMR stipulated its identity as "discovering common elements and universal principles among different material fields and creating new materials science which can predict new functions," and proposed a new research strategy, "mathematics-materials science collaboration." Prof. Motoko Kotani, a mathematician, was newly appointed as Center Director in FY2012. Under her leadership, AIMR quickly organized a system for mathematics-materials science collaboration. AIMR cleared the two-year careful observation by making "remarkable progress beyond expectation" within two years. Based on such highly motivated measures, AIMR has pursued world-leading research, published 1,852 papers including 47 papers appearing in Science, Nature, and Nature's sister **<u>[ournals</u>**, and received internationally-acclaimed awards such as the American Physical Society's Oliver E. Buckley Condensed Matter Prize, Humboldt Research Award, and IEEE David Sarnoff Award. These indicate that AIMR has already achieved "World Premier Status."

AIMR's challenge <u>attracts talented researchers from around the world</u>, making it an international research center. Around 50% of researchers or more are from overseas (from 28 countries). The official language is English and research support is substantial. AIMR is pursuing joint research with 15 institutions, establishing joint laboratories in the University of Cambridge and the University of California, Santa Barbara (UCSB), and a system to accelerate joint research. Administrative staff have acquired the skills for international services such as exchange agreements with overseas institutions, helping make AIMR <u>a hub of global brain circulation</u>.

On system reform, AIMR has achieved <u>independence from the university and top-down</u> <u>decision-making by the Center Director</u>. Besides English services, thorough support for researchers allows them to start research almost immediately. These efforts have created <u>ripple</u>

effects through the host institution. Tohoku University is establishing the "Organization for Advanced Studies" modelled on AIMR. Administrative services in English is being institutionalized throughout the university. SATOMI VISION, the president's action plan, stipulates "an open research environment based on flexible personnel system," "establishment of a Promotion Office for operation reform," and "an administrative system providing services in English throughout the university" after AIMR. Task Forces and Working Groups have also been organized and AIMR's experiences have become a driving force for promoting the system reform and internationalization of the whole university.

II. Items

1. Overall Image of Your Center

AIMR was established to pursue (1) creating new materials with innovative functions that surpass existing ones, (2) constructing devices based upon new fundamental paradigms, and (3) promoting applied research projects on materials and establishing systems that will contribute to society by building a foundation for safe and enriched livelihoods. These are conducted by our world-leading organization for interdisciplinary research through an innovative method of atomic and molecular control departing from traditional approaches. After the FY2011 Interim Evaluation, AIMR stipulated its identity as "discovering common elements and universal principles among different material fields and creating new materials science which can predict new functions" (extract from the modified Research Center Project accepted in late FY2011), and proposed a new research strategy, "mathematics-materials science collaboration" injecting mathematical viewpoints into materials science to create new materials science. Prof. Kotani, a mathematician, was appointed as Center Director in FY2012 to meet this challenge. Under new leadership, AIMR quickly organized a system for mathematics-materials science collaboration, setting up the Mathematics Unit, the Interface Unit and three Target Projects. AIMR published high-quality emerging results in *Science* and <u>Physical Review Letters</u> within the limited period of two years by injecting mathematical viewpoints. This significantly elevated the standing of the Center, receiving favorable evaluations, such as "remarkable progress beyond expectation." mathematics-materials science collaboration at an institutional level is unprecedented, attracting great interest from the materials science and mathematics communities. AIMR has both prepared a world-leading research environment and strengthened its partnership network with world-leading overseas institutions. Thus AIMR functions as a hub for international joint research and global brain circulation. The facts above and the descriptions below indicate that AIMR has already achieved "World Premier Status".

2. Research Activities

AIMR researchers are constantly producing basic and applied research of the highest quality and impact in the materials science field. For about six and a half years following the

Center's establishment, the number of publications has increased steadily. AIMR researchers have published 1,852 papers, with 47 papers appearing in Science, Nature, and Nature's sister journals. Other papers were also published in high-impact journals such as Proceedings of the National Academy of Sciences of the United States of America (PNAS), Physical Review Letters (PRL), Journal of the American Chemical Society (JACS), and Advanced Materials. Full-time researchers are often invited to international meetings, giving about 100 invited presentations per year. Since AIMR's establishment, researchers have received international and domestic scientific awards for their achievements, including Arthur C. Cope Scholar Award of the American Chemical Society, James C. McGroddy Prize for New Materials of the American Physical Society, Oliver E. Buckley Condensed Matter Prize of the American Physical Society, the International Rubber Conference Organization Medal, Centenary Prize of the Royal Society of Chemistry, Humboldt Research Award, Presidential Early Career Award for Scientists and Engineers, the IEEE David Sarnoff Award, and the Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology (MEXT). The synergistic effect of having leading researchers under one roof has increased total external research funds. AIMR researchers obtained 2.3-3.4 billion yen per year or 5-8% of the entire external research funds of Tohoku University. These noteworthy awards and large funding indicate that AIMR's research activities are visible on the global research stage.

3. Interdisciplinary Research Activities

Since FY2009, AIMR has conducted the "Fusion Research Proposal Program" to provide start-up funding to about 20 accepted proposals every year, giving researchers a chance to start new interdisciplinary fusion research. In late FY2010, AIMR proposed a new strategy, "mathematics-materials science collaboration," to accelerate fusion research. Researchers held intensive discussions throughout FY2011 on how to achieve materials science and mathematics collaboration. Then, in FY2012, a mathematician was appointed as Center Director and AIMR was reorganized as the first institute in the world to promote mathematics-materials science collaboration at an institutional level. After establishing the Mathematics Unit, composed of mathematicians, AIMR employed eight young researchers in theoretical physics, theoretical chemistry and applied mathematics to bridge the gap between mathematicians and materials scientists. Such researchers belong to the newly-established Interface Unit. AIMR set three target projects (1) Non-equilibrium Materials based on Mathematical Dynamical Systems, (2) Topological Functional Materials, and (3) Multi-Scale Hierarchical Materials based on Discrete Geometric Analysis to provide researchers with a common and concrete image of the goal of mathematics-materials science collaboration. The synergistic effect of these efforts has greatly accelerated fusion at AIMR. Shortly thereafter, some emerging results have already appeared as articles co-authored by materials scientists, mathematicians and theoretical physicists published in journals such as Science and Physical Review Letters. The introduction of mathematical viewpoints has also accelerated fusion among materials scientists.

4. International Research Environment

Since establishing the Center, the proportion of researchers from abroad has steadily increased. This has been kept at around 50% or more. AIMR completed the common equipment room, where even short-stay visitors can start experiments almost immediately. AIMR has conducted joint research with 15 partner institutions. 14 are overseas institutions. In particular, AIMR forged a closer relationship with three institutions as satellites; University of Cambridge, UCSB, and Institute of Chemistry, Chinese Academy of Sciences. AIMR has set up joint laboratories at the University of Cambridge and UCSB, and a system for accelerating joint research. The *International Relations Unit* of the Administrative Division is contributing greatly to promoting researcher exchange between AIMR and overseas institutions and steadily making AIMR a hub of global brain circulation by pursuing exchange agreements and operating original exchange programs, such as GI³ (Global Intellectual Incubation and Integration) Laboratory Program and Brain Circulation Program.

5. Organizational Reforms

On system reform, <u>AIMR has achieved both independence from the university and top-down decision-making by the Center Director</u>, thus AIMR's path can be quickly and flexibly decided and managed. Besides English services in the Administrative Division, thorough support for researchers allows them to start research immediately after arrival. These efforts have created <u>ripple effects through the host institution</u>. Tohoku University is establishing the "Organization for Advanced Studies" modeled on AIMR. The standard for international services in English for the whole university is now progressing. SATOMI VISION, the president's action plan, stipulates "an open research environment based on flexible personnel system," "establishment of a Promotion Office for operation reform," and "an administrative system providing services in English throughout the university" after AIMR; Task Forces and Working Groups have been organized for this purpose and <u>AIMR's experiences have become a driving</u> force for promoting the system reform and internationalization of the whole university.

6. Others

Common Equipment: The "Common Equipment Unit" was established to prepare the "Common Equipment Room," which contains some common equipment useful for many of the AIMR researchers, and to coordinate the renting of apparatuses held by AIMR laboratories or common equipment within the university. Furthermore, a researcher (assistant professor) with a Ph.D. degree and high-level research skill was appointed as manager of the unit, and a research environment has been realized in which even researchers from abroad or researchers freshly arrived can start their research quickly.

Graduate School of Spintronics: Tohoku University plans to establish a Graduate School of Spintronics, where AIMR researchers will play a central role and world-leading researchers and graduate students will gather.

World Premier International Research Center Initiative (WPI) Progress Report of the WPI Center (For Extension Application Screening)

Host Institution	Tohoku University	Host Institution Head	Susumu Satomi
Research Center	Advanced Institute for Materials Research (AIMR)	Center Director	Motoko Kotani

^{*} Write your report within 30 pages. (The attached forms are in addition to this page count.) Keep the length of your report within the specified number of pages.

Common Instructions:

- * Please prepare this report based on the current (31 March 2014) situation of your WPI center. * Use yen (¥) when writing monetary amounts in the report. If an exchange rate is used to calculate the yen amount, give the rate.
- 1. Overall Image of Your Center (write within 2 pages including this page)

Describe the Center's current identity and overall image. For centers that have had a change in their directors, describe that transition and the effects of the change.

On the sheets in Appendix 1, list the Principle Investigators and enter the number of center personnel, a chart of the center's management system, a campus map showing the center's locations on the campus, and project funding.

Since FY2007, AIMR has united and tackled the creation of new research fields through world-leading science expertise, internationalization, system reform and interdisciplinary fusion, achieving "world premier status." AIMR's prior advancements and present status follows.

AIMR was established to pursue (1) creating new materials with innovative functions surpassing existing ones; (2) constructing devices based upon new fundamental paradigms; and (3) promoting applied research projects on materials and establishing systems that will contribute to society by building a foundation for safe and enriched livelihoods. These are all conducted by our world-leading organization for interdisciplinary research through an innovative method of atomic and molecular control departing from traditional approaches (extract from the Research Center Project proposed in 2007). Despite the FY2011 Interim Evaluation stating "AIMR research results are excellent," AIMR was asked to clarify its identity as a WPI Center, which was beyond its existing scope. In response, AIMR stipulated its identity as "discovering common elements and universal principles among different material fields and creating new materials science which can predict new functions" (extract from the modified Research Center Project accepted in late FY2011), and proposed a new strategy, "mathematics-materials science collaboration;" injecting mathematical viewpoints into materials science in order to create new materials science. Prof. Motoko Kotani, a mathematician, was appointed Center Director in FY2012 to meet this challenge. The WPI Program Committee recognized this exciting challenge; however, the committee approved AIMR for a second five-year term on the condition that AIMR's activity be carefully observed for two years (FY2012-FY2013) with respect to mathematics-materials science collaboration in both academic research and management terms (extract from the report for Interim Evaluation and FY2010 Follow-up Report by WPI Program

Committee, December 2011).

Under new leadership, AIMR quickly organized a system for the mathematics-materials science collaboration, setting up the Mathematics Unit, the Interface Unit and three Target Projects. <u>AIMR cleared the two-year careful observation by making "remarkable progress beyond expectation" within two years</u>, through, for example, publishing high-quality papers that appeared in *Science* and *Physical Review Letters*, by injecting mathematical viewpoints (extract from the *FY2013 Follow-up Report* by WPI Program Committee, January 2014). Presently at AIMR, mathematicians and experimental scientists conducting research together can discuss problems directly and make new models. Experimentalist immediately evaluate the models based on experiments, sending the data to the mathematicians who then can modify the models. Through positive feedback loops, AIMR continues to embark on the challenge of increasing the predictability of materials science. <u>Collaboration like this at an institutional level is unprecedented, attracting great interest from the materials science and mathematics communities.</u>

AIMR pursued <u>world-leading research</u> based on such highly motivated measures for creating new materials science on the basis of prediction through discovering commonalities and universal principles among different fields. From October 2007 to December 2013, they have published 1,852 papers, including 47 in *Science, Nature*, and *Nature's sister journals*; and internationally-acclaimed awards such as *the American Physical Society's Oliver E. Buckley Condensed Matter Prize*, the Humboldt Research Award, and the IEEE David Sarnoff Award, indicating that <u>AIMR has already achieved "World Premier Status."</u>

AIMR's challenge attracts talented researchers from around the world. It has become an international research center whose ratio of overseas researchers hovers around 50% or more (from 28 countries). The official language is English, with complete research support. AIMR pursues joint research with 15 institutions (14 overseas, 1 domestic), and has established joint laboratories at the University of Cambridge and the University of California, Santa Barbara, completing the system. The International Relations Unit set in the Administrative Division is pursuing international services by concluding exchange agreements with overseas institutions and promoting researchers exchange. AIMR thus <u>functions as a hub for global brain circulation</u>.

On system reform, AIMR has achieved both independence from the university and top-down decision-making by the Center Director, thus AIMR's path can be quickly and flexibly decided and managed. Besides English services at the administrative office, thorough support for researchers allows them to start research immediately after arrival. These efforts have spread.over.AIMR's host institution, Tohoku University. The Organization for Advanced Studies, promoting rejuvenation of the entire university, will be established, based upon AIMR. The standard for international services in English for the whole university is now progressing. **SATOMI VISION**, the president's action plan, stipulates "an open research environment based on flexible personnel system," "establishment of a Promotion Office for operation reform," and "an administrative system providing services in English throughout the university" after AIMR. Task Forces and Working Groups have been organized for this purpose, becoming a driving force for system reform and internationalization of the whole university.

2. Research Activities (within 15 pages)

2-1. Research results to date

Describe issues of a global level that the Center has challenged, and give the results. Select 20 representative results achieved during the period from 2007 through March 2014. Number them [1] to [20] and provide a description of each. Place an asterisk (*) in front of those results that could only have been achieved by a WPI center.

• In Appendix 2, list the papers underscoring each research achievement (up to 40 papers) and provide a description of each of their significance.

AIMR research achievements are characterized as the hierarchical structure from the basic science of observing atoms/molecules to applications which can contribute to society, such as creating new materials and device development, indicating complete fusion within our center. The following twenty descriptions are the representative research results achieved at AIMR, arranged from basic to applications, also corresponding to the structure and function of materials in terms of scale, from micro to macro. See **Appendix 2-1** for details of the original papers.

[Observe and understand atoms and molecules]

AIMR holds world's best and unique equipment developed by researchers, observing materials on the atomic/molecular level.

*[1] Direct observation of atoms on an oxide surface

Observing oxide surfaces with atomic resolution using scanning tunneling microscopy (STM) is very difficult. Oxide materials are fundamentally electrically insulating, and they are not appropriate for STM observations using tunneling current. Even if the films are thin, it is extremely difficult to make atomically flat oxide films, thus few papers have reported atomic images of oxide surfaces in spite of their importance for electronics. Since the basis for research at AIMR is direct observation of atoms and molecules and complete understanding of the relationship between atoms/molecules and properties of materials, we tried to develop advanced STM with the world's highest resolution to facilitate the direct observation of oxide atoms, which are promising materials for next-generation electronics (see also "2-2. Research environment including facilities and equipment"). A pulsed laser deposition (PLD) system and a combined metal evaporation cell and an oxygen gas source system were attached to the STM apparatus in order to obtain epitaxial oxide films with atomically flat surfaces. Thanks to such efforts, researchers have successfully obtained clear images of oxide materials such as SrTiO₃ and TiO₂ and wide-gap semiconductors such as β-Ga₂O₃, which are attracting attention as new electronic devices, and LiCoO₂ for lithium ion batteries. This system also enables investigation of the electronic structure of each atom with scanning tunneling spectroscopy (STS). (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 1, 2 Published in ACS Nano, Physical Review Letters)

*[2] Observation of the arrangement of atoms near grain boundaries

The structure of grain boundaries in polycrystalline materials plays an important role in determining the material's properties and functions. Therefore, an atomic-level understanding of the grain boundaries is crucial for creating new functional polycrystalline materials. AIMR researchers have succeeded in obtaining images of arranged atoms and segregated impurity atoms at their interface by improving measurement techniques with scanning transmission electron microscopy (STEM), and comparing the experimental data with the results of the first principle theoretical calculation. More specifically, they managed to directly observe the lattice distortion in layered oxide thin films containing lanthanum, strontium, titanium, etc., and to elucidate their electronic properties. They also developed a new technique for investigating the atomic structure and phenomena along grain boundaries using artificial "bicrystals," consisting of two crystals cut along different crystallographic directions. Using these, they discovered the segregation of impurity elements like calcium and titanium, and how dislocation along grain boundaries is formed. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 3-5 Published in **Nature, Nature Communications**)

*[3] Elucidation of electronic structures by spin-ARPES with world's highest resolution "Dirac cone" as the common band dispersion to novel materials

AIMR researchers developed a spin- and angle-resolved photoemission spectrometer (spin-ARPES) with the world's highest resolution by attaching a Mott detector for spin detection. Using such advanced equipment, they have measured the precise electronic band structures of various materials with novel physical properties, such as superconductors and topological insulators, and discovered the mechanisms behind them. They measured graphite intercalation compound C_6 Ca with higher superconductivity transition temperature (T_c) of 11.5 K, finding that the energy gap specific to the superconductivity is identified in the interlayer band located between the carbon atomic layers. They also studied an iron-based high-temperature superconductor BaFe₂As₂, revealing that it has a characteristic Dirac cone electronic structure, where a pair of conical bands meet at the top near the Fermi level in a very similar manner to graphene. The Dirac cone band dispersion has also been observed in topological insulators by this group, suggesting that the Dirac cone is universal and ubiquitous for graphene, iron-based superconductors, and topological insulators. These results were introduced in Physics Today (April 25, 2011) under the title "Fashionable physics." (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 6-9 Published in Nature Physics, **Physical Review Letters**)

*[4] Mapping the mechanical characteristics of polymers with AFM

It is necessary to understand the relationship between atomic/molecular level structures and macro-scale properties for the creation of new materials that AIMR aims for. AIMR researchers have developed a technique for two-dimensionally mapping mechanical properties like adhesiveness and stiffness (Young's modulus) on a nanometer-micrometer scale area using an atomic force microscope (AFM). Macro-scale mechanical properties can now be discussed based on molecular level properties. This AFM measurement technique can be applied to measuring the micro-viscosity distribution of bulk metallic glass (BMG) as described in the section "3.

Interdisciplinary Research Activities" in this report, and largely contributed to the fusion research at AIMR and elucidation of a common structure behind the different kinds of amorphous materials such as polymer glass and BMG. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 10 Published in **Macromolecules**)

*[5] Elucidation of atomic structures in metallic glasses

It had long been thought that the atomic structure of bulk metallic glasses (BMG) was random and had no long-range order. However, using the latest techniques, AIMR researchers revealed that the atomic structure of BMG is not completely random and has some typical clusters, sometimes leading to mid- or long-range ordering. Such atomic-scale un-uniformity is considered to be effective in improving glass-formation performance. Recently, Zircon-Nickel-based BMG was observed with a scanning transmission electron microscope (STEM), where electron diffraction patterns from atomic clusters with narrow electron beams were obtained. This indicates that BMG consists of atomic clusters in short-range order. Mathematicians joined this study afterward, applying computational homology analysis, revealing that the geometric distortions of icosahedral clusters in metallic glass can be scaled up to long-range disorder in a simple manner with topological connectivity. Thanks to their efforts, AIMR researchers resolved the underlying discrepancy which remained unsolved for half a century, reaching a milestone in the structural analysis of BMGs by applying advanced experimental techniques and mathematics to this field. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 11-14 Published in Physical Review Letters, Nature Materials, Science)

[Control atoms and molecules]

AIMR Researchers derive functions based on atomic/molecular-level understanding.

*[6] Oxide electronics: superconductivity and fractional quantum Hall effect

Oxide electronics is a field that has grown rapidly since the early years of AIMR. In particular, researchers around the world acknowledge AIMR's discoveries of superconductivity induced by field effect carrier doping and the fractional quantum Hall effect in oxide materials. Oxide materials are fundamentally insulators and nonconductive, but they have some advantages such as their stability, their abundance in the Earth's crust, and their low cost. AIMR researchers obtained the following outstanding results by controlling the charge carrier: (1) changing insulator oxides (SrTiO₃, KTaO₃, etc.) into superconductors with high-density carrier doping using an electric double layer, (2) realizing high-luminance zinc oxide (ZnO) light-emitting diodes by developing a p-type ZnO semiconductor with high carrier mobility, and (3) confirming the fractional quantum Hall effect in oxide materials for the first time by preparing a high-quality interface between a magnesium oxide zinc thin film and a zinc oxide substrate. Recently, by utilizing oxides' transparency, AIMR researchers have also succeeded in creating transparent superconductor thin films using spinel lithium titanate oxide (LiTi₂O₄). (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 15-18 Published in Nature Materials, Nature Nanotechnology, Applied Physics Letters)

*[7] Spintronics : Controlling "spin"

Tohoku University has a widely-recognized spintronics program. Top-level researchers in spintronics from around the world gather at AIMR and develop "spin-centered science" from basic science to applications related to "spin." The Prof. Emeritus T. Miyazaki and Assoc. Prof. S. Mizukami group is known as a pioneer in "tunnel magnetoresistance (TMR)," discovering the high TMR ratio at room temperature. Prof. H. Ohno and Prof. T. Dietl are known as pioneers in "magnetic semiconductors." Prof. E. Saitoh is known as a forerunner in "spin current," pioneering the "inverse spin Hall effect" and the "spin Seebeck effect." In collaboration with Prof. G.E.W. Bauer, Prof. Saitoh is expanding the field of "spin caloritronics". Prof. T. Takahashi, at the forefront of measuring properties of materials, developed spin-ARPES (see [3]) with the world's highest resolution, making it possible to visualize the electronic structures of spin-related materials such as superconductors and topological insulators. At AIMR, such world-class researchers are performing advanced research in spintronics. Recently progress has been made in developing a technique to measure accurate spin currents, energy transport using magnetic waves, spin polarization due to the Rashba effect, and controlling the current leakage in topological insulators. The achievements by Prof. Miyazaki and Prof. Mizukami Group will be described in [17]. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 19-22 Published in Nature Materials, Nano Letters, Nature Communications)

*[8] Phonon engineering: Controlling "lattice vibration"

A phonon is a quantized state of lattice vibration related to thermal conductivity. There is a general tendency for thermal conductivity to be proportional to electric conductivity (Wiedemann-Franz law), thus thermal conductivity is often disguised by electric conductivity. However, in recent years, some exceptional materials that do not correspond to such tendencies have been found in the materials groups, such as clathrates having nano space (cages) which can encapsulate different atoms. In clathrates, different atoms so encapsulated display free motion called "anharmonic rattling phonons." This motion decreases thermal conductivity through the increase of phonon scattering, though electrical conductivity stays high. This property brings an advantage to thermoelectric materials. Based on comparing two types of clathrates, $Ba_{24}Si_{100}$ and $Ba_{24}Ge_{100}$, it was also found that such properties are useful for developing high T_c superconductors. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 23 Published in **Physical Review Letters**)

*[9] Dynamics between two surfaces and solid/liquid interface

AIMR has a special technique to investigate a force acting between two surfaces. In general, atomic force microscopy (AFM) is used to measure the force; however, in this case, the force between the surface (plane) and top of the tip (point), is measured, not between planes. AIMR researchers have developed brand-new equipment to measure surface force by gradually decreasing the distance between two surfaces. This also can measure friction by applying shear stress (see also "2-2. Research environment including facilities and equipment"). In addition, AIMR has theoretically evaluated the experimental results. They performed a molecular

dynamics simulation of ionic liquids sandwiched between two hydroxylated silica surfaces. The study revealed how the shape of ionic liquid molecules influences their layering structure of positive- and negative-charged layers, and how the layered structure of nanoconfined liquids determines their mechanical properties. This result qualitatively explains viscosity change of confined ionic liquids. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 24 Published in **Physical Chemistry Chemical Physics**)

*[10] Controlling polymerization

It is considerably difficult to obtain single polymer crystals, long viewed as a challenge, because their long and flexible backbones tend to get tangled, forming structures with no long-range order. Researchers at the AIMR joint research center at University of California, Santa Barbara succeeded in making single polymer crystals based on a revolutionary idea. They grew single crystals made up of monomers, subsequently making monomers in the crystals polymerize with the coming monomers with visible light, marking the first time that the quantitative conversion of a small molecule to a macromolecule was achieved with visible light. The polymer can be reversibly decomposed into monomers, is very strong, and can be removed individually from the crystals, leading to various applications. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 25 Published in **Science**)

[Create new materials]

Various materials have been created based on the results of fundamental research, some only made possible by the interdisciplinary fusion teams at AIMR.

*[11] Metallic glass nanowire

In general, one-dimensional structured materials are crystalline with numerous defective points such as dislocations, point vacancies, twins, and grain boundaries. These are the starting points of deterioration, as well as the active spots in chemical reactions. AIMR researchers have succeeded in creating nanowires using superplastic deformation, characteristic to metallic glass at high temperatures. Since these nanowires have no defective points, their lengths can be extended. In addition, in fusion research with the micro electro mechanical system (MEMS) laboratory, the resonance measurement of metallic glass nanowires has revealed the elasticity modulus at nano-levels, suggesting applications for nano-resonators. Recently, this research group has also discovered a new, cost-effective technique for producing metallic glass nanowires in bulk. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 26 Published in **Advanced Materials**)

[12] Organic/inorganic hybrid nanocrystals

Green materials should be ecological both in function and process. AIMR researchers developed new materials using supercritical "water" as a reaction solvent, paving the way for creating multi-functional hybrid materials without hazardous chemical substances. Supercritical conditions enable organic materials and inorganic materials to mix, leading to the expression of

multiple functions. For example, an organic/inorganic hybrid flexible plastic film containing 90% or more boron nitride fine particles simultaneously shows high thermal conductivity, insulation, and adhesion, which are normally incompatible. Researchers also succeeded in creating CeO₂ nanocrystals surrounded by (100) surfaces, which show the highest catalytic activity for cleaning automobile emissions through surface modification with organic molecules under supercritical hydrothermal conditions. Such new hybrid materials combining several normally incompatible characteristics are called "super hybrid materials." This research was introduced in **Physics Today** (February 16, 2011) under "Molecules to materials." (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 27 Published in **Nano Letters**)

*[13] Nanoporous metals for highly efficient catalysts and supercapacitors

Nanoporous metals created by dealloying are attracting great interest for various applications. AIMR researchers have reached two big milestones with nanoporous metals: one is an application for highly-efficient catalysts, the other an application for supercapacitors. AIMR researchers found that nanoporous gold enhances the oxidation reaction of organic silane compounds at room temperature. The main advantage to conventional particle type catalysts is that nanoporous metal catalysts can be reused multiple times without degrading their catalytic properties, while particles have a short life owing to agglomeration. In the application for supercapacitors, AIMR researchers used nanoporous gold as a cage encapsulating manganese dioxide (MnO₂) which can store charges at metal sites through an electron transfer process called "pseudocapacitance," succeeding in improving charging/discharging speeds and energy density. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 28, 29 Published in **Angewandte Chemie International Edition, Nature Nanotechnology**)

*[14] Ultra-hard ceramics

Substantial progress was also made in ceramics development. The brittleness of ceramics mainly stems from grain boundary properties. Ceramics are commonly made by sintering compressed powders at a temperature just below their melting point, generating various crystal grain structures which may act as fracture initiation points. In this study, AIMR researchers lowered the sintering temperature of boron carbide under high pressure conditions, obtaining crystallites with uniform grain sizes. In such specimens, thin amorphous carbon layers coat the crystal grains and help in lubrication. This is a breakthrough mechanism for reducing the brittleness of ceramics, challenging notions that "ceramics are brittle." (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 30 Published in **Nature Communications**)

*[15] Biomaterials

AIMR has also begun contributing to the biomaterials field, based on AIMR's strong point of investigation on the atomic/molecular level. For example, AIMR researchers are focusing on creating fibrous microstructures to be used as muscle tissue and ultra-thin sheets facilitating the transplant of cells and tissues to a human body. Being fundamental material, a good scaffold providing cells a place to adhere to and multiply, as well as long-term viability is needed. AIMR researchers selected a semi-natural hydrogel material gelatin methacrylate

(GelMA) for this, confirming it was a suitable material to guide cells, trap them, and make them retain long-term viability. AIMR researchers also developed ultra-thin polymer "nanosheets" supporting cell growth and transplantation at a specific location. These results not only increase AIMR's strong points, but create a new way to contribute to society. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 31, 32 Published in Lab on a Chip, Advanced Materials)

[Create new devices and systems]

Various devices/systems have been developed to give AIMR's achievements back to society.

[16] Energy materials and devices

Creating materials and devices for "energy harvesting" and "energy saving" are among AIMR's final goals. To this end, AIMR set up a target project "Core Technology for Nano Energy Devices," and promoted development of new materials and devices. One step is breaking down the theoretical Shockley–Queisser (S–Q) limit in Si-based solar cell efficiency with a quantum dot (QD). The well-aligned QD superlattice is expected to form minibands between the valence band and the conduction band, inducing an extra two-photon-transition. AIMR researchers confirmed the efficacy of this strategy and with theoretical simulations, predicted that they could realize a maximum efficiency of 50.3%. AIMR also promoted development of new complex hydrides for energy conversion, storage, and transport. In particular, AIMR researchers focused on ABX₃ perovskites, succeeding in elucidating their formation process using *in situ* synchrotron X-ray diffraction measurements for the first time ever. The three-step reaction they discovered is a leap for future applications. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 33, 34 Published in Nanotechnology, Applied Physics Letters)

*[17] Memory device using tunnel magnetoresistance (TMR)

Magnetoresistive random access memory (MRAM), notable as nonvolatile memory that contributes to energy-saving, uses tunnel magnetoresistance (TMR), technology pioneered by AIMR researchers, as storage elements. To realize gigabit-class MRAM, a perpendicular magnetization magnetic thin film with both high spin polarization and strong perpendicular magnetic anisotropy is necessary. However, suitable materials have not been found so far. In this study, AIMR researchers focused on manganese gallium alloy, finding that this material satisfies the requirement, expecting its practical application. They are also attempting to discover new prospects with organic materials. Since it is believed that electron spin can be preserved long-term and electrons can, in principle, travel long distances without flipping their spin, they constructed spin valve devices using fullerene (C₆₀) films with various thicknesses, and observed travelling up to a record-high distance of 110 nanometers for magnetoresistance at room temperature. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 35, 36 Published in **Physical Review Letters, Nature Communications**)

*[18] Biomimetics: hierarchical structures and functions

Living things endured endless structural variations during evolution, retaining those best suited to their environment, indicating that learning from nature is a shortcut to design and create new functional materials in harmony with natural environments. AIMR placed high priority on "Biomimetics," succeeding in creating a new biomimetic surface by self-organization consisting of a metal—polymer hybrid structure that both repels and absorbs water. A non-equilibrium phenomenon (water droplet evaporation) is used to fabricate surface microstructure, surface function (to repel and absorb water droplets) is produced by the topological effect of the microstructure, and multifunction (repelling and absorbing) is caused by hierarchical structure. This important research is closely tied to three projects for AIMR's mathematics and materials science collaboration. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 37 Published in Chemistry of Materials)

*[19] Bio-imaging and bio-sensing devices

As described in "Biomaterials", the importance of biological application is increasing in materials science. Besides creating new biomaterials, developing observational tools for imaging and sensing the biological phenomena with high resolution is required. AIMR researchers have developed a high-resolution, non-invasive imaging method called voltage-switching mode scanning electrochemical microscopy (VSM–SECM), succeeding in simultaneously acquiring high-resolution topographical and electrochemical images of living cells. Their next challenge is to monitor release-related changes in neuron topography. Their other achievement is developing a high-density integrated electrochemical device to monitor stem cells. They quantified cellular activity from embryoid bodies on the array by collecting local current signals based on "redox cycling." Using this device, they succeeded in finding signs of stem cell differentiation. Therefore, the device is considered to be useful for screening embryoid bodies' differentiation levels. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 38, 39 Published in **Proceedings of the National Academy of Sciences USA, Angewandte Chemie International Edition**)

*[20] Micro Electro Mechanical System (MEMS)

While MEMS has been one of the strongest subjects for application research at Tohoku University for some time, further advancement has been achieved through interaction with researchers from various disciplines. AIMR researchers are primarily working to develop packaging technology, succeeding recently in developing wafer-level packaging using nanoporous metals. They have also made achievements in developing optical scanners using bulk metallic glass (BMG) thin film, making an optical scanner suitable for very small (approximately 1 mm) endoscopes by creating a metallic glass thin film by sputtering. This technology utilizes the superior mechanical properties of metallic glass, such as its strength. These tools will also play important roles in maintaining industrial infrastructures and enabling long and safe system operation, leading to saving natural resources and energy. MEMS technology is central to realizing a sustainable green society by introducing new, functional green materials into devices created by fusion research at AIMR. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 40 Published in **Optics Letters**)

Many papers have been published in extremely high-impact journals such as *Science*, *Nature* and *Nature's sister journals*; and in the highest-ranked journals in materials science, physics, applied physics, chemistry, device engineering, and comprehensive/multidisciplinary fields, such as *Advanced Materials*, *Physical Review Letters (PRL)*, *Applied Physics Letters (APL)*, *Journal of the American Chemical Society (JACS)*, *Lab on a Chip*, *Proceedings of the National Academy of Sciences of the United States of America (PNAS)*. The number of papers appearing in *Science*, *Nature* and *Nature's sister journals* are shown below for reference (only papers showing an author as affiliated with AIMR).

	2007	2008	2009	2010	2011	2012	2013
Science		1		1	2		3
Nature					1		
Nature Communications				1	2	2	7
Nature Materials		1	2	2	2	3	5
Nature Nanotechnology			1		2	1	1
Nature Physics			2	1	1	1	1
Nature Photonics						1	
Sum total	0	2	5	5	10	8	17

2-2. Research environment including facilities and equipment

Describe the degree to which the Center has prepared a research environment appropriate for a world premier international research center, including facilities, equipment, and support systems; and describe the functionality of that environment.

AIMR has prepared the following facilities and equipment appropriate for a world top-level research center. AIMR has also prepared equipment necessary for all researchers at the Common Equipment Unit in the Research Support Center, completing the system for generous support.

Scanning tunneling microscopy (STM) with extremely high resolution: According to the institute's identity, direct observation of atoms and molecules is the basis for creating new functional materials. During construction of the AIMR main building, the experimental area was structurally disconnected with the office area in order to insulate the experimental area from vibrations. Concrete was placed directly on the bedrock after removing the thick soil, and an STM with an extremely low temperature apparatus was set on a dual noise-cancelling system placed on the concrete. Thus, the STM system with the world's highest resolution was completed. As described in 2-1. Research results to date [1], researchers have succeeded in observing accurate electronic structures of oxide surfaces and thin films using STM.

Spin- and angle-resolved photoemission spectroscopy (spin-ARPES) with the world's highest resolution: Accurately measuring the electronic structure of materials is important for understanding their properties. In particular, AIMR is making extensive efforts to build up "Spin-centered Science," so that spin- and angle-resolved photoemission spectroscopy

(spin-ARPES), which provides information about band structure and "spin," plays a crucial role. AIMR researchers have developed spin-ARPES with the world's highest resolution, succeeding in obtaining the precise band structures of many superconductors, including iron-based superconductors and topological insulators, drawing a great deal of attention.

World's only apparatus for surface force measurement: The study of friction draws great attention nowadays, since friction is closely linked to energy problems. However, it has been difficult to understand the atomic/molecular-level mechanism of friction because of the lack of techniques to directly measure the interaction between two contact surfaces. AIMR researchers developed a technique to measure accurately the attractive and repulsive force between them with a precise measurement of the inter-surface distance. The force is measured with decreasing the distance or applying a shear force between surfaces. This advanced technique now plays a major role in friction research.

Mapping of the mechanical characteristics of polymers with AFM: AIMR researchers have developed a technique to map mechanical properties such as viscosity and stiffness in a nanometer scale area using an atomic force microscope (AFM). While this measurement technique using AFM was developed for polymer materials research, it can apply to measurements such as the micro-viscosity distribution of bulk metallic glass (BMG), and has largely contributed to the fusion research at AIMR, as well as elucidating the common structure underlying different kinds of amorphous materials, such as polymer glass and BMG.

Supercritical hydrothermal synthesis system: New techniques for material synthesis broaden possibilities for exotic materials. AIMR researchers developed a supercritical hydrothermal synthesis technique which can combine two hitherto unmixed substances, such as water and oil, making it possible to produce nanoparticles of metal oxides, sulfides, and nitrides; and to modify the nanoparticle surfaces with organic molecules. These have been successfully applied, developing highly-efficient catalysts and flexible ceramics with high thermal conductivity.

Common Equipment Room which is the most convenient for researchers in the world: As shown in the "organization chart" in Appendix 1-3, AIMR established the "Common Equipment Unit" in the "Research Support Center." This unit consists of three parts (Part 1, 2, and 3). Part 1 indicates the "Common Equipment Room" owned by AIMR in their main building. This room has a field emission scanning electron microscope (FE-SEM) with a spatial resolution of around 1 nm and an energy-dispersive spectrometer (EDS) attached, a multifunctional X-ray diffraction (XRD) applicable to any sample type, a Laue camera, X-ray photoelectron spectroscopy (XPS), a high resolution Raman microscope with three laser wavelengths, thermal analysis (TG-DTA, DSC), an absolute PL quantum yields measurement system, optical microscopes, and machine tools. Part 2 is a system to ask AIMR laboratories to provide some apparatuses for common use. Part 3 is a system that facilitates use of equipment of other departments. These facilities and systems are managed by two technical staff members, one a researcher holding a Ph.D. degree, who maintain all the equipment and help researchers to use the equipment in Part 1. They also deal with all arrangements with respect to Part 2 and Part 3. An ideal research environment has been completed, thanks to their efforts and careful support.

Even overseas researchers can begin experiments the moment they arrive at AIMR.

2-3. Competitive and other funding

Describe the results of the Center's researchers to date in securing competitive and other research funding.

• In Appendix 2, describe the transition in acquiring research project funding, and note any external funding that warrants special mention.

As shown in **Appendix 2-2** in detail, the amount of external research funds (sum of competitive and noncompetitive funds) increased steadily with the interactions of talented researchers at AIMR. While the amount was 0.64 billion yen (for half a year) in the year of AIMR's establishment, in the second year, the amount increased to 2.08 billion yen (FY 2008). In the third year, the amount further increased to 2.37 billion yen (FY 2009). After the fourth year, more than 2.3 billion yen has been accumulated (3.45 billion yen in FY2013). This amount corresponds to **5-8%** of the total amount of the external funds of Tohoku University as a whole. The number of researchers (assistant professors and above) at AIMR (~70) is about 2.4% of that of the whole of Tohoku University, and the ratio of researchers from abroad is higher than that of other departments. Therefore, a value of 5-8% is enough to express how great of an amount of external research funds the AIMR researchers obtain.

This ample budget means the best researchers who can obtain not only Grants-in-Aid for Scientific Research, but also the biggest projects, are gathering at AIMR. For example two PIs, Prof. Masayoshi Esashi and Prof. Hideo Ohno, won the Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST Program) and conducted their projects until the end of FY2013. Prof. Hiroyuki Isobe (PI) won the Exploratory Research for Advanced Technology (ERATO) research funding program, starting his project from the end of FY2013 in the AIMR main building. There are other several projects which were or still are being carried out by AIMR PIs. These include the Strategic Basic Research Programs (CREST), Green Network of Excellence (GRENE), and projects supported by New Energy and Industrial Technology Development Organization (NEDO). Large scale research projects are actively promoted.

There has been significant progress on foreign researchers acquiring external research funds. For example, Prof. Mingwei Chen, AIMR PI, won the Strategic Basic Research Programs (**CREST**) in FY2011. Other successful examples since AIMR was established include a young foreign researcher succeeding in obtaining the Grants-in-Aid for Scientific Research under the guidance of a mentor of the Researcher Support Office, Research Support Center, AIMR.

2-4. State of joint research

Describe the results of joint research conducted with other research organizations both in and outside Japan.

Most great-impact papers from AIMR were produced by joint research with other research organizations both in and outside Japan. AIMR researchers published 1,852 papers from October 2007 through December 2013. Among those, 601 (32.9%) were results from collaborations with

domestic research institutions excepting Tohoku University, and 713 (38.5%) were results of international collaboration. In other words, 70% or more papers were the results of joint research with organizations in and outside Japan. Aside from the fusion research inside the Center, AIMR researchers have carried out numerous joint research projects with other institutions in and outside Japan. This contributed to not only improving the quality of papers, but also increasing AIMR's international presence.

2-5. Appraisal by society and scientific organizations

Describe how society and/or scientific organizations in and outside Japan have recognized the Center's research achievements.

In Appendix 2, list awards received and invitational lectures given by the Center's researchers.

As listed in **Appendix 2-3**, AIMR researchers have received many internationally-acclaimed awards, such as the Oliver E. Buckley Condensed Matter Prize of the American Physical Society, the Humboldt Research Award, and the IEEE David Sarnoff Award. Researchers have also given many talks, including numerous plenary addresses and keynote lectures in international conferences and international research meetings. Three AIMR PIs (Prof. Mingwei Chen, Prof. Takashi Takahashi, and Dr. Ali Khademhosseini) have been selected as Thomson Reuters Highly Cited Researchers 2014, indicating remarkable achievement since AIMR was established seven years ago. AIMR is highly recognized in the world not only for its individual researchers, but also its research center. For example, AIMR activities were once focused on by THE ACADEMIC EXECUTIVE BRIEF (ISSN 2212-0424), published twice yearly by Elsevier, focusing solely on limited authoritative institutions. According to these accomplishments, it is clear that AIMR and AIMR researchers are highly-regarded internationally in society and scientific organizations.

2-6. Feeding research outcomes back into society

2-6-1. Applications of research results

Describe the applications created from research results, their effect in spawning innovation, intellectual properties (IPs) obtained, and joint research activities conducted with corporations, etc.

The goal of AIMR is contributing to the welfare of mankind through the creation of new materials sciences, which can design new materials based on theory; and creating new functional materials and new devices/systems. Therefore, during the past seven years AIMR has made considerable effort to spawn innovation and cooperation with industries, as well as fundamental research. Some representative examples of innovation creation projects which AIMR's PIs acquired, IPs, and joint research activities with corporations and their outcomes are listed below:

Innovation Creation Projects:

- Creation of Innovation Centers for Advanced Interdisciplinary Research Areas Program (FY2007-FY2013); total budget 2,959 million yen (PI Prof. Masayoshi Esashi)
- · Project for intellectual production collaboration promotion and innovation, "Creation of new

industry and international base of intellectual production collaboration systems based on supercritical nanomaterial technology;" total budget 414 million yen, consortium of 76 companies (PI Prof. Tadafumi Adschiri)

- Ministry of Economy, Trade and Industry Innovation Promotion Project, "Creation of Core Technologies for Advanced Energy Devices through Vertically-Integrated Technologies and New System of Industry-Academia Collaboration;" total budget 360 million yen, consortium of 32 companies (PI Prof. Seiji Samukawa)
- Center of Innovation (COI), "The center of innovation for creation of platform on big life data from unconscious sensing to support human and social well-being;" budget 577 million yen for FY2013, 1,949 million yen for FY2014-15, undecided for FY2016-21 (Research Leader: PI Prof. Tomokazu Matsue)

Intellectual properties (IPs):

- Terunobu Miyazaki and Shigemi Mizukami. "Magneto-resistive element and magnetic memory." <u>US Patent</u>, US8520433 Apr. 27, 2013.
- Tadafumi Adschiri. "Production of Nano Metal Sulfide Particles by Supercritical Hydrothermal Synthesis." Filing date: September 1, 2008 Appl. No.: 2008-223244 Patent No.: 5115983
- Dmitri V. Louzguine. "Method for producing a metallic glass nano-particles aggregate." Filing date: June 10, 2011 Appl. No.: 2011-130026 Kokai (unexamined patent publication) No.: 2012-255197
- Koji S. Nakayama. "Metallic glass nanowire manufacturing method, metallic glass nanowire manufactured thereby, and catalyst containing metallic glass nanowire." Filing date: April 17, 2012 International Appl. No.: PCT/JP2012/060309 International unexamined patent publication (Kokai) No.: WO2012/147559 A1
- Hideo Ohno. "Nonvolatile logic integrated circuit." Filing date: April 25, 2012 Appl. No.: 2012-099785 Kokai (unexamined patent publication) No.: 2013-229721
- · Many others

Joint research activities conducted with corporation and applications created from research results:

Prof. Masayoshi Esashi is a central and leading researcher in MEMS (Micro Electro Mechanical Systems) technology in Japan, spanning fundamental research to industrial applications. He and his co-workers have developed not only core and fundamental technologies for MEMS, but have also established an open-access facility named the "hands-on access fabrication facility" that companies can easily access and utilize for prototyping or small volume production. So far, they have established an industry-academia-government cooperation organization, "MEMS Park Consortium," of which more than sixty companies, universities, local governments, and public organizations are members, raising the standard of MEMS technologies in Japan and the Tohoku

region. Based on longstanding collaboration with Fraunhofer-Gesellschaft, Germany, they established the Fraunhofer Project Center at AIMR, succeeding in forming a global network. In addition, they have started an Industrial-Academic Partnership collaboration laboratory at AIMR with DENSO Corporation. They play a leading role in returning research results to society.

Prof. Tadafumi Adschiri and co-workers have developed supercritical hydrothermal synthesis technology to efficiently produce nanoparticles of metal oxides, sulfides, and nitrides, and have used this technology to develop manufacturing equipment, succeeding in the development of practical applications. A tubular flow reactor and a batch-wise reactor were developed in cooperation with Itec Co. Ltd. and AKICO Ltd., respectively, and brought into manufacture and sales. They also pioneered an organic surface modification technique to disperse nanoparticles into solvents and polymer matrixes. The practical applications of these technologies were implemented as a national project (five-year program from FY2007 with total research expenses of ~3 billion yen) by congregating 11 industrial companies. Prof. Adschiri received many awards for these achievements, including the Merit Award for Industry-Academia-Government Collaboration (Minister of MEXT Award) and National Invention Award.

Prof. Terunobu Miyazaki, **Assoc. Prof. Shigemi Mizukami** and co-workers (Mizukami laboratory since FY2013) collaborated with Toshiba Corporation to realize nonvolatile magnetic memory MRAM (magnetic random access memory), as pioneers first in the world to discover the tunnel magnetoresistance (TMR) at room temperature experimentally. In FY2011, Toshiba Corporation established the basic technique to fabricate gigabit-class spin-transfer torque MRAM which satisfies both requirements for small writing current and large MR ratio. This collaboration team is continuing robust collaborative studies to realize practical G bit class MRAM technology.

The pulse-modulated plasma which **Prof. Seiji Samukawa** invented has become standardized technology for the plasma etching process in semiconductor devices, and is growing to be a technology used worldwide. Prof. Samukawa and co-workers have advanced the practical application of this technology, and it has been equipped as standard in Lam Research and Applied Materials' inductively coupled plasma (ICP) equipment. Recently, Tokyo Electron's dual-frequency parallel-plate technology has also been added to etching equipment. Pulse-modulated plasma will be indispensable to the future creation of devices. This technology is expected to contribute to the production of about half of the devices of the world's total market size. In addition, 12-inch Neutral Beam Apparatus has been developed with Tokyo electron Co., Ltd. in 2012-13, and an apparatus will be installed in Tohoku University in FY2014.

Prof. Shin-ichi Orimo and co-workers are pursuing the research and development of new power storage devices, such as all-solid-state rechargeable batteries, using complex hydrides based on the fusion research at AIMR using the synthesis of complex hydrides and the laboratory's original technologies for turning the hydrides into devices. By collaborating with Mitsubishi Gas Chemicals Company, Inc., they succeeded in premiering the operation of such batteries, resulting in six patent applications and adoption of the research proposal to JST-ALCA (Leader: Dr. A. Unemoto). These achievements largely contributed to the establishment of an Industrial-Academic Partnership Project in AIMR with Hitachi, Ltd., where they will tackle

challenges such as realization of higher energy density as power storage devices.

2-6-2. Achievements of Center's outreach activities

If the Center has conducted its own unique outreach activities, describe those worthy of special mention.

In Appendix 2, list and describe media coverage, press releases, and reporting.

As shown in detail in **Appendix 2-4** and **2-5**, AIMR has made great efforts in outreach activities and media coverage. Although the General Affairs Section of the Administrative Division managed public relations (PR) for the first couple years, Dr. Susumu Ikeda was appointed as the first "outreach manager" in April 2010, and AIMR started systematic outreach activities. Besides issuing the outreach magazine "TOHOKU WPI Tsu-Shin", AIMR ran booths introducing AIMR's research activities at various scientific events, such as **Sendai-Miyagi Science Day**, **Tohoku University Open Campus**, **Katahira Festival** and **Tohoku University Festival**, in which high school students and general citizens participate. AIMR's outreach team also joined scientific events such as the **Science and Technology Festa in Kyoto**, **WPI Joint Symposium**, and **AAAS Annual Meeting**, together with other WPI centers' outreach teams. AIMR held the "**Idea Contest – Challenger to the Future**" jointly with MANA, collecting ideas about materials from students of primary, junior high, and high schools and technical collages, and praised excellent ideas after strict judgment by the committee. The commendation ceremony and exhibition of the awarded ideas were held at the National Museum of Nature and Science in Ueno.

In April 2012, Dr. Yasufumi Nakamichi was appointed as AIMR outreach manager. The PR & Outreach Office was further strengthened with its integration into the International Relations Unit of the Administrative Division. Dr. Nakamichi completely reformed the AIMR website and pamphlets, stating he would issue a new outreach magazine, "AIMR MAGAZINE," composed of timely interviews, research topic introductions, event reports, researcher introductions, and high-quality impact photos. In December 2013, under Dr. Nakamichi, AIMR succeeded in holding the WPI joint symposium "Science Talk Live 2013 by WPI" at the Sendai International Center. Five researchers from WPI centers gave TED-like presentations in the first stage, and four teams of high school students (three from Super Science High School in Miyagi Prefecture and one from Maryland, U.S.A.) presented their research results in English in the second stage. Success was possible through accumulated experiences of outreach activities over a couple of years and the cooperative relationship with high schools formed through various joint events. For example, international exchange events were held between students from SSH and core-SSH-related high schools and AIMR researchers (mainly overseas researchers) at AIMR every year. We provide students an opportunity to speak in English to overseas researchers with earned reputation.

The PR & Outreach Office asked AIMR laboratories to increase press releases by promising support for manuscripts, and tentatively initiated <u>overseas-targeted press releases</u>. As a result, many research results have appeared in the media, mainly in newspapers as shown in **Appendix 2-5**. International publications such as "SpringerBriefs in Mathematics" and "Mathematics for Materials Research" (Editor-in-Chief M. Kotani) also contributed to increasing AIMR's presence.

3. Interdisciplinary Research Activities (within 3 pages)

3-1. State of Strategic (or "Top-down") Undertakings toward Creating New Interdisciplinary Domains

Since FY2009, AIMR has provided the "Fusion Research Proposal Program" to help researchers promote interdisciplinary fusion research between/among different research groups. So far, 94 proposals have been accepted (13, 14, 17, 10, 18, and 22 proposals in FY2009 (first half), FY2009 (latter half), FY2010, FY2011, FY2012, and FY2013, respectively), and funds were provided for the launch of new fusion research between/among different research groups. In FY2012, mathematics—materials science collaboration was started in earnest, and the number of accepted fusion research projects increased to support the initial stage of such collaborations. Researchers who were provided fusion research funds were offered an opportunity to present results from their projects at Tea Time the next year, so that results could be shared with other researchers and inspire more new ideas for the next fusion.

In FY2012, under the leadership of the new Center Director (mathematician) and new AIMR Administrative Director (theoretical physicist), achieved great mathematics-materials science collaboration which started at the end of FY2010, and its basis was almost completed in FY2011. The Mathematics Unit established in March 2011 now consists of two PIs (Professor Yasumasa Nishiura, the leader of the unit, and Professor Motoko Kotani) and five assistant professors. After the establishment of the Mathematics Unit, we noticed that we need researchers who can bridge the gap between mathematicians and materials scientists. Mathematicians and materials scientists use different terminology, and it was very difficult to understand each other in a short amount of time. Therefore, AIMR established the Interface Unit in FY2012. Eight independent young theoretical physicists and chemists and applied mathematicians with a mathematical background and also knowledge of materials science were selected through international recruitment. Interface Unit researchers play the role of interpreter and bridge the gap between the mathematicians and materials scientists as well as conducting their own research.

In late FY2011, AIMR set three **Target Projects**, (1) Non-equilibrium Materials based on Mathematical Dynamical Systems, (2) Topological Functional Materials, and (3) Multi-Scale Hierarchical Materials based on Discrete Geometric Analysis, in order to provide researchers a shared, concrete image of the goal of the mathematics—materials science collaboration. The Interface Unit effectively interacted with these Target Projects. Due to this, opportunities for exchange between researchers with different backgrounds increased, and AIMR is now ready to step up to the next stage where we can develop higher quality science. The role of the interface researchers has gradually changed into leading the interdisciplinary fusion research on their own initiative, and some papers have been submitted from the interdisciplinary teams. It is necessary that there be reciprocal benefit; that is, mathematics develops by this collaboration, and materials science advances as well per the injection of mathematics. Although this challenge will take time, results are beginning to be steadily produced.

The interdisciplinary fusion has evolved at AIMR as schematically shown in **Figure 1**. AIMR was established in FY2007 and four groups, Bulk Metallic Glasses, Material Physics, Soft Materials, and Device/System, were organized. It was difficult for these groups to intermingle with each other initially. After the launch of the "Fusion Research Proposal Program" in FY2009, researchers started to have opportunities to meet researchers from different groups and discuss fusion research. They jointly applied the proposal of fusion research and carried out research for one year. This effectively enhanced communication between/among different groups, and overlap between the groups gradually and partially proceeded. Mathematics—materials science collaboration began in the end of FY2010, and the Mathematics Unit and Interface Unit were established. With the injection of mathematics, which provides common language to all disciplines, and the activity of young theoreticians who bridged the gap between experimental materials scientists and mathematicians, the boundaries between groups have almost disappeared. Now AIMR is filled with an atmosphere in which researchers can discuss new research, regardless of the collaborators' disciplines.

With the Joint Seminar as a formal seminar of the whole center, the seminars and study meetings of each Target Project, the mathematics—materials science joint seminar together with the Applied Mathematics Forum (AMF), Tohoku University, Friday Tea Time, and other small seminars frequently and suitably maintain the heated atmosphere for fusion without attenuation. In order to share plans and results of each target project from the entire Center, the **Target Project—Interface Unit (TP—IU) Joint Forum** is held every 3-4 months.

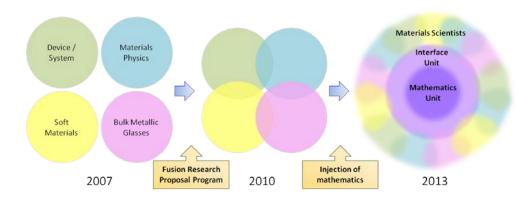


Figure 1 Evolution of interdisciplinary fusion at AIMR.

3-2. State of "Bottom-up" Undertakings from the Center's researchers toward Creating New Interdisciplinary Domains

Interdisciplinary fusion at AIMR is supported not only by the center's top-down promotion but also by the spontaneous "bottom-up" activities of the researchers themselves. In particular, daily meetings and discussions held spontaneously by researchers are the driving force enhancing fusion. By pure coincidence, at AIMR, the injection of mathematics and Great East Japan Earthquake occurred around the same time. Thanks to the synergistic effect of mathematics injection and a change of values and perspectives due to the earthquake, the habit of

spontaneously holding meetings and discussing new challenges spread throughout the Center. Although it goes without saying that the most important thing in fusions is their own will to achieve, people tend to become passive due to large risks. However, the current AIMR is able to boldly tackle fusion in spite of the many risks. This status is largely due to the researchers' spontaneous actions to achieve real fusion, and the voluntary discussions or changes in attitudes caused from such a background. The key to accomplishing the mathematics—materials science collaboration is to find themes challenging for both materials scientists and mathematicians. Fortunately, there is an environment at AIMR to discuss that substantially.

3-3. Results of research in fused research fields

Describe the Center's record and results by interdisciplinary research activities.

• In Appendix 3, list the main papers published (up to 20 papers) on the Center's interdisciplinary research and provide a description of each of their significance.

AIMR has conducted various fusion research as listed below, and has started to obtain some emerging results based on the mathematics–materials science collaboration. In particular, mathematicians and theoreticians of the Interface Unit largely contributed to papers 1-6. See **Appendix 3** for details.

- 1) Elucidation of metallic glass structure by computational homology (Science)
- 2) Stoichiometry control based on a mathematical model (Physical Review Letters)
- 3) New geometric measures for finite carbon nanotubes (Pure and Applied Chemistry)
- 4) Mathematical technique predicts molecular magnet (Proceedings of the Royal Society A)
- 5) Deformation analysis of BMG with a stochastic model (Journal of alloys and compounds)
- 6) Effect of spin Hall magnetoresistance on spin pumping (Applied Physics Express)
- 7) Nanoscale mechanical heterogeneity in a metallic glass (Physical Review Letters)
- 8) Nanoporous gold for effective catalysts (Angewandte Chemie International Edition)
- 9) The atomic structure of nanoporous gold surface causing catalysis (Nature Materials)
- 10) Nanoporous gold reductive catalysts (Journal of the American Chemical Society)
- 11) Metallic glass Pd-catalyst with skeleton nanopores (Chemical Communications)
- 12) Bilayer graphene C₆Ca (Proceedings of the National Academy of Sciences USA)
- 13) Reduced graphene oxide for phototransistors (ACS Nano)
- 14) Electrically induced ferromagnetism in cobalt-doped titanium dioxide (Science)
- 15) Metallic glassy nanowires and application to nanoresonators (Advanced Materials)
- 16) Functional micromirror using Fe-based metallic glass (Optics Letters)
- 17) Controlling carbon nanotube alignment in hybrid hydrogels (Scientific Reports)
- 18) Nanoporous gold based high-sensitive optical sensor of mercury ions (ACS Nano)
- 19) New organic semiconductor BPFT for OLETs (Journal of Materials Chemistry C)
- 20) Theoretical analysis of BPFT's light emission (The Journal of Physical Chemistry C)

4. International Research Environment (within 4 pages)

4-1. International Circulation of Best Brains

4-1-1. Center's record of attracting and retaining top-world researchers from abroad

Describe the participation of top-world researchers as PIs and the residing of joint researchers at the Center.

• In Appendix 4, give the number of overseas researchers among all the Center's researchers, and the yearly transition in their numbers.

With regard to statistical data, as shown in **Appendix 4-1**, the number of researchers from abroad increased smoothly, and almost reached the number of the final goal in the third year (FY2009) since the establishment of AIMR. Additionally, from the viewpoint of ratio, the ratio of researchers from abroad to the total number of researchers has stayed around 50% or more since FY2009. AIMR invited the world's top researchers to AIMR as Principal Investigators (PIs) and Junior PIs, listed below. Furthermore, by utilizing the GI³ (Global Intellectual Incubation and Integration) Laboratory Program and with the cooperation of PIs, Junior PIs, and overseas adjunct professors/associate professors, AIMR has promoted the exchange of researchers, and so far many researchers have stayed at AIMR and carried out joint research.

[Bulk Metallic Glasses (BMG) Group]

Prof. A. Lindsay Greer: Former head of the Department of Materials Science and Metallurgy, University of Cambridge. He has carried out long-standing collaboration with Prof. Dmitri V. Louzguine (PI, AIMR). Dr. Jiri Orava (postdoc at Cambridge joint laboratory) is now moving forward with the joint research between them. Prof. Greer himself stays at AIMR for joint research several weeks every year.

Prof. Alain Reza Yavari: Professor of Grenoble Institute of Technology. Winner of the Award for Scientific Excellence, French National Center for Scientific Research (CNRS), 2011. He stays at AIMR 1-3 months every year, and carries out joint research with Mingwei Chen's (PI, AIMR) and Dmitri V. Louzguine's (PI, AIMR) groups on bulk metallic glasses. Dr. Konstantinos Georgarakis (assistant professor) is placed at Yavari's laboratory at AIMR to enhance joint research.

[Materials Physics Group]

Prof. Alexander Shluger: Professor of University College London. He has his laboratory at AIMR and places Dr. Filippo Federici Canova (postdoc). Dr. Shluger stays at AIMR several weeks every year and is carrying out joint research with the Kazuto Akagi (Associate Professor, AIMR) group, the Kazue Kurihara (PI, AIMR) group and the Dmitri Louzguine (PI, AIMR) group on theoretical calculation, surface physical chemistry, and metallic glasses, respectively. He also places young researchers, including Ph.D. students of his laboratory at University College London, at AIMR as visiting scientists.

Prof. Paul S. Weiss: Director of California NanoSystems Institute (CNSI), UCLA. Distinguished Professor of Chemistry and Biochemistry & Materials Science and Engineering, UCLA.

Editor-in-Chief of ACS NANO. He is carrying out joint research with the Taro Hitosugi (associate professor, AIMR) group on atom/molecule control of surface and interface. He has his laboratory at AIMR and places Dr. Patrick Han (assistant professor) at the AIMR laboratory, and has arranged a joint research structure with AIMR.

Prof. Qi-Kun Xue: Professor and Vice President of Tsinghua University. He places Dr. Ling Zhang (assistant professor) at AIMR, and performs joint research to develop sensors using nanoporous metals which the Mingwei Chen (PI, AIMR) group creates, and the surface physics technique of the Xue group.

[Soft Materials Group]

Prof. Thomas P. Russell: Professor of University of Massachusetts Amherst. Director of Energy Frontier Research Center (EFRC). Silvio O. Conte Distinguished Professor. He stays at AIMR 2-5 weeks out of every year and is carrying out joint research with the Ken Nakajima (associate professor, AIMR) group on polymers and soft materials. He places young researchers, including Ph.D. students of his laboratory at the University of Massachusetts, at AIMR as visiting scientists.

Prof. Li-Jun Wan: Former Director of the Institute of Chemistry, Chinese Academy of Sciences. Fellow of Chinese Academy of Sciences. One of the world authorities on surface chemistry. Dr. Zhe Chen (postdoc) is placed at Wan Laboratory at AIMR, and is doing joint research on molecular nanotechnology.

In FY2013 **Prof. Kosmas Prassides**, Professor of Durham University and an authority of molecular superconductors, joined AIMR. He will be a full-time PI of AIMR from FY2014.

[Device/System Group]

Prof. Thomas Gessner: Professor of Chemnitz University of Technology. Director of the Fraunhofer Research Institution for Electronic Nano Systems (ENAS) in Germany. He is conducting joint research on micro electro mechanical systems (MEMS) with Prof. Masayoshi Esashi (PI, AIMR) based on their long collaboration. Dr. Yu-Ching Lin (associate professor) and Dr. Yao-Chuang Tsai (postdoc) are placed at Gessner's laboratory at AIMR and they have arranged a joint research structure. He also places young researchers, including Ph.D. students of his laboratory at Chemnitz University of Technology, at AIMR as visiting scientists. Due to such strong cooperation, the AIMR - Fraunhofer Project Center has been established, and further joint research is carried out. We are planning to extend our contract to a more comprehensive one.

Junior PIs: AIMR also assigned three talented world-leading young researchers, **Prof. Ali Khademhosseini** (associate professor of Harvard Medical School), **Prof. Winfried Teizer** (associate professor of Texas A&M University), and **Prof. Hongkai Wu** (associate professor of Hong Kong University of Science and Technology), to be "Junior PIs". They have a laboratory at AIMR, and employ three or four assistant professors and postdoctoral researchers. These three Junior PIs stay at AIMR several months a year, and by utilizing video meetings, they manage the laboratory and conduct their research.

In addition to PIs and Junior PIs, many other researchers, including adjunct professors, adjunct associate professors, and visiting professors, stayed at AIMR and carried out joint research. As a new case using "AIMR Brain Circulation Program" which was started in FY2013 to further promote global brain circulation with the cooperation of other departments of Tohoku University, **Dr. Pawel Hawrylak** (Principal Research Officer of National Research Council of Canada, Humboldt Research Award winner in 1999) stayed at Prof. Yoshiro Hirayama (AIMR Affiliated Professor) Laboratory and published a joint research paper with AIMR in *Physical Review B*. AIMR's global network is spreading through various type of joint research.

4-1-2. Employment of young researchers at the Center and their job placement after leaving the Center

Describe the Center's employment of young researchers, including postdoctoral researchers, and the positions they acquire after leaving the Center.

- In Appendix 4, enter the following:
 - The state of international recruitment for postdoctoral researchers, applications received, and selections made
 - The percentage of postdoctoral researchers from abroad
 - The positions that postdoctoral researchers acquire after leaving the Center

The recruitment of postdoctoral researchers (research associates at AIMR) has always been international, propagated by posting information on the AIMR website and well-known scientific journals such as *Nature* and *Science*. As a result, AIMR can employ excellent young researchers from 18 countries around the world, leading to fruitful research results. As shown in **Appendix 4-2**, the number of applicants increased considerably with the rise in AIMR's international reputation, and the ratio of successful to total applicants is now less than 10%. As shown in **Appendix 4-3**, many of the postdoctoral researchers come from abroad. Since its establishment, AIMR has employed 109 postdoctoral researchers in total (see **Appendix 4-4**). Among these, 80 researchers (73% of total) are from overseas.

From the viewpoint of brain circulation, as listed in **Appendix 4-4**, the researchers have obtained higher positions after their experience at AIMR as a postdoctoral researcher for a couple of years. Many of them have been appointed as assistant professors at universities, while some have even become full or associate professors.

- 4-1-3. Overseas satellites and other cooperative organizations
- In Appendix 4, describe the state of the Center's agreements concluded with overseas satellites and other cooperative organizations.

Agreements are listed in **Appendix 4-5**. AIMR is conducting collaborative research with 15 partner institutions, 14 of them being overseas institutions. In particular, AIMR arranged a closer relationship with three institutions as satellites; the University of Cambridge, the University of California, Santa Barbara (UCSB), and the Institute of Chemistry, Chinese Academy of Sciences. AIMR has set up joint laboratories at Cambridge and UCSB, and established a system for accelerating international joint collaborations. Postdoctoral researchers at AIMR have been

employed and placed at the joint laboratories as shown below. They ordinarily work at the joint laboratories while sometimes coming to AIMR, staying at counterpart laboratories to discuss joint research.

PI or Adjunct Professor	Joint Lab Researcher	Counterpart at AIMR		
Cambridge				
Prof. A. Lindsay Greer (BMG)	Dr. Jiri Orava	Prof. Dmitri V. Louzguine		
Dr. Erwin Reisner (Chemistry)	Dr. Katherine Orchard	Prof. Tadafumi Adschiri		
		Prof. Naoki Asao		
G. R. Grimmett (Mathematics)	Dr. Demeter Kiss	Prof. Motoko Kotani		
UCSB				
Prof. Fred Wudl (Organic device)	Dr. Yonghao Zheng	Prof. Katsumi Tanigaki		

4-2. Center's record of holding international symposia, workshops, research meetings, training meetings and others

In Appendix 4, describe the main international research meetings held by the Center.

AIMR has held international research meetings as listed in **Appendix 4-6**. The annual "AIMR International Symposium (AMIS)" (called "WPI-AIMR Annual Workshop" before 2012) is held yearly in February or March, gathering more than 1,400 attendees from over 15 countries (in total of seven years). In addition, AIMR has frequently held joint workshops with overseas partner institutions, including satellites. These activities largely contributed to AIMR's international recognition. Furthermore, AIMR plays a central role in Tohoku University's international events, such as Tohoku University Day (held in China and U.K.) and the German-Japanese University Consortium (HeKKSaGOn).

4-3. System for supporting the research activities of overseas researchers

Describe the Center's preparations to provide an environment conducive for overseas researchers to concentrate on their work, including for example living support in various languages or living support for their families.

Based on the objectives of the WPI program, the Administrative Division, of which 90% or more of staff members can provide service in English, was first established; and all office documents were translated into English. In addition, AIMR tackled housing problems, making efforts to support overseas researchers' housing, such as preferential entrance to university accommodation. AIMR set up the Researcher Support Office from late FY2011, manning support staff near the laboratories, and starting advanced support for daily life.

4-4. Others

Describe the Center's policy for sending Japanese researchers overseas to gain international experience, and give examples of how the Center is working to create career paths for its researchers within a global environment of researcher mobility.

GI³ Laboratory Program was basically designed to invite overseas researchers to AIMR. In FY2013, AIMR started a converse program to send AIMR researchers, including Japanese, to partner institutions abroad for several weeks or months. So far, 9 researchers have utilized this dispatch program.

5. Organizational Reforms (within 3 pages)

5-1. Decision-making system in the center

Describe the strong leadership that the director is giving the Center's operation and its effect, and the division of roles and authority between the Center and its host institution.

AIMR has made efforts to achieve organizational reforms. The management under the top-down decision-making by the Center Director made it possible to determine orientation and strategy quickly and flexibly. This was a truly significant reform for the Japanese university system. Thanks to this, mathematics-materials science collaboration has progressed smoothly within a very short period of time. If a parliamentary system, such as faculty meetings, remained, AIMR could not start such challenges so quickly and achieve emerging results within just two years.

An Executive Committee, consisting of the Center Director, administrative director, and group leaders appropriately advises the Director before her important decision, so as to keep the robust advancement of AIMR as an institute for materials science that assembles researchers from various fields. Furthermore, the <u>International Advisory Board</u> (holds yearly meetings) and the <u>External Advisory Board</u> set up in FY2013 have given AIMR very important advice for making AIMR the world's top research center.

Although AIMR is a department in Tohoku University, it is completely independent from the host university except for the assignment of the Center Director. The Director has made all personnel decisions concerning PIs and researchers.

5-2. Arrangement of administrative support staff and effectiveness of support system

Describe the assignment of the Center's administrative support staff who have English language and other specialized skills, effort made in establishing the support system, and the system's effectiveness.

In order to remove the language problem, a consistent barrier for researchers from overseas, the Administrative Division, where 90% or more of staff <u>can provide services in English</u>, <u>was first</u> established, and <u>all office documents were translated into English</u>. Thanks to this effort, even the researchers from overseas, who account for about 50% of all researchers at AIMR, can concentrate on their research without any inconvenience.

"The International Relations Unit" set up in the Administrative Division started the international services which were previously performed by researchers, such as <u>concluding</u> exchange agreements with overseas institutions, support for holding international meetings, promoting researchers' exchange, and support for foreign researchers for applying for external research funds. With this progress, researchers are able to further concentrate on their research. Since the Public Relations (PR) and Outreach Office are involved in the International Relations Unit, AIMR can effectively conduct PR and outreach activities both domestic and overseas.

Based on the success of internationalization at AIMR, Tohoku University stipulated "an administrative system which can provide service in English throughout the university" in the

SATOMI VISION, the president's action plan, and has started preparations.

5-3. System reforms advanced by WPI program and their ripple effects

Concisely itemize the system reforms made to the Center's research operation and administrative organization, and describe their background and results. Describe the ripple effects that these reforms have on the host institution. (Describe the ripple effects on other institutions.)

- Posting staff who can provide English service (90% or more), aiming for internationalization
 of the administrative office. Translation of all official documents into English. Prior
 negotiations for concluding exchange agreements by the administrative staff belonging to
 the International Relations Unit.
 - <ripple effect> A briefing session was held introducing AIMR's international administrative works to the whole university. Based on this achievement, making an "administrative system providing services in English throughout the university" was stipulated in SATOMI VISION. This achievement in AIMR's Administrative Division has become a driving force of the globalization of administration throughout the university.
- Establishment of a Research Support Center consisting of a "Common Equipment Unit," a
 "Computation-Aid Unit," a "Mathematics Collaboration Unit," and a "Researcher Support
 Office (Mentor + Secretarial staff)," aiming to provide the best research environment and
 daily support. Establishment of joint appointment employment to invite talented researchers
 from abroad.
 - <ripple effect > The president of Tohoku University has established a "Project Team" for discussing strategies to make the university a hub of global brain circulation based on AIMR's research support system and employment system.
- Completion of know-how and logistics for arranging international meetings and inviting overseas researchers by the Administrative Division (mainly International Relations Unit).
 <ripple effect> The accumulated logistics expertise led to the establishment of the "Tohoku Forum for Creativity" in FY2013. In FY2014, the expertise will be inherited by the "Research Reception Center" to be set up in the "Organization for Advanced Studies" as an organization for helping researchers to come and stay in Sendai.

5-4. Support by Host Institution

The following two items concern the support that the host institution provides the Center, including those items of support that it committed to at the time of the initial project proposal submittal or in its revised commitment following the project's interim evaluation. Describe the functional measures that the host institution has taken to sustain and advance the Center's project.

- 5-4-1. Record of host institution support and its effects
- In Appendix 5, describe the concrete measures being taken by the host institution.

The commitment made by former President Akihisa Inoue at the time of the initial project proposal submittal, and its revised commitment following the project's interim evaluation, has been inherited by the current President Susumu Satomi since FY2012 and upheld. See **Appendix 5-1** with regard to the concrete measures being taken by the host institution.

Thanks to these measures, AIMR can quickly advance system reforms in personnel, salary, preparing research environments, and research strategies of the Center (accelerating interdisciplinary fusion by mathematics—materials science collaboration) by top-down decision-making by the Director, without any restriction by conventional university rules. Such an ideal environment has brought about visible outcomes.

5-4-2. Position of the Center within the host institution's mid-term plan

• To Appendix 5, attach the cover sheets of the host institution's "Mid-term objectives" and/or "Mid-term plan" and parts of these documents related to the WPI Center.

The "Mid-Term Plan" of Tohoku University (extracts of the pages relating to AIMR) is attached as **Appendix 5-2**. There are three clear statements about WPI and AIMR in the second interim plan (from April 1st, 2010 to March 31st, 2016) of the "Mid-term plan" as follows:

- ➤ "Conduct education programs for fostering skilled researchers in interdisciplinary fields in cooperation with the Institute for International Advanced Research and Education, Advanced Institute for Materials Research (AIMR), and Global COE Program."
- ➤ "Strengthen and support AIMR, which was launched with the adoption by the World Premier International Research Center Initiative (WPI), to develop AIMR into a world-leading international research network hub."
- ➤ "Promote innovative research by making use of the Institute for International Advanced Research and Education, AIMR, Graduate School of Biomedical Engineering, among other institutes of Tohoku University."

5-5. Others

Describe efforts advanced to foster young researchers (e.g., start-up funding, autonomous research environment) and to enlist female researchers.

• In Appendix 5, give the transition in the number of female researchers.

Over the past seven years, AIMR promoted six young researchers (associate professors) to Junior PIs through a peer-review process by an international evaluation committee, and provided them research space and personnel expenses nearly the same as those of PIs, so that they can pioneer new research areas. Furthermore, to promote mathematics—materials science collaboration, AIMR employed 13 young theoretical researchers as Mathematics Unit and Interface Unit members. They were also provided with an independent research environment, so as to create new research plans by joining up with any experimental researchers and mathematicians based on their own ideas, and develop a new approach to our goal. Since FY2009, AIMR has provided the "Fusion Research Proposal Program" to help, in particular, young researchers make opportunities to talk to researchers from other fields and start interdisciplinary fusion research based on their own ideas, not necessarily those corresponding to the laboratory's research orientation. As shown in **Appendix 5-3**, the ratio of female researchers is 9% (6% for PI and 10% for other researchers) at present.

6. Others

• In addition to the above 1-5 evaluation items, only if there is anything else that deserves mention regarding the center project's progress, please note it.

Common Equipment: Although the "Common Equipment Unit" has already been described above in the text, AIMR's common equipment system, which was designed based on thorough analysis of the researchers' needs through a questionnaire sent to all the laboratories, etc. and provides the most effective support, also receives many inquiries from outside the university.

Graduate School of Spintronics: Tohoku University plans to establish a Graduate School of Spintronics, where AIMR researchers will play a central role and world-leading researchers and graduate students will gather.

Salary system: A new salary system was established that pays PI allowance and merit-base wage depending on the result of a performance evaluation at the end of every fiscal year. This new salary system at AIMR gave rise to the creation of the "Distinguished Professor System" at the host institution, Tohoku University.

Overseas traveling expenses: In order to increase convenience for the invited foreign researchers and simplify paperwork, AIMR realized liquidation denominated in foreign currencies concerning charges forward for overseas traveling expenses. Furthermore, AIMR has developed a new system to send airline tickets directly to foreign researchers.

Secretary manual: The Secretary Part Office Work Manual (Secretary manual) was developed mainly by Researcher Support Office staff from the Research Support Center, from the viewpoint of researcher support. This manual has been used as a reference for establishing researcher support systems in other departments.

Overseas training of administrative staff: AIMR's Administrative Division established the Overseas Training Program and started dispatching administrative staff to overseas institutions to learn about administration and research support systems. In FY2014, we plan to invite administrative staff from overseas institutions (from the Carnegie Institution for Science in June, and from the University of Chicago in September). Such invitations provide learning opportunities not only for dispatched staff, but also for all administrative members.

Tea Time: In order to increase opportunities for personal communication among researchers, including foreign PIs, "Tea Time Talk (small seminar by overseas senior researchers)" and mini-concerts during Tea Time have been started, in addition to ordinary Tea Time held on every Friday. These events are producing a good atmosphere at the Center.

Reform of sense of the administrative staff: Reforming the sense of the administrative staff members is another important factor of AIMR's success. Staff members are conscious of the importance of their roles, and take the lead in opening new ways to realize internationalization in a Japanese institute.

7. Center's Response to Results of FY2013 Follow-up (including Site Visit Results)

[Suggestion 1]

A discussion of the long-term future strategy of materials science at AIMR is recommended. It is important for AIMR to hold the current strategy with full confidence. Also short- and medium-time strategy should be carefully prepared in parallel.

[Response]

As field of crystallography advanced on the basis of geometry and group theory, it is evident that mathematics has influenced various disciplines such as materials science and induced innovation in each period. This historical fact also proves that interaction between mathematics and other fields gradually matured into new scientific fields over many mathematics-materials science collaboration should be the challenge we tackle over the long-term. AIMR has started to obtain some emerging results through the mathematics-materials science collaboration, which was made possible by support from the WPI program for ten years, much longer than general projects. The mathematics-materials collaboration is beneficial only when it has continued long years without any interruption, such as project breaks. The commitment by the host institution, Tohoku University, to sustain AIMR as a permanent department guarantees AIMR's long-term challenge, and it is greatly appreciated. On the other hand, as the WPI Program Committee suggested, it is also important to prepare short- and medium-time strategies in parallel. In particular, young researchers who play a central role in making steady progress on the challenge have to achieve something during their term of office that lasts for a couple of years, before moving on to their next position. Thus, it is quite important to be successful at both encouraging accomplishments of young researchers within a short office term and mathematics-materials science collaboration requiring the span of a few decades. The director emphasized, when she began conducting the mathematics-materials science collaboration, that we should first start the collaboration with fields that suit mathematics and gradually expand out; we should also not forget to simultaneously continue our world top-level materials science we have created so far, because AIMR is not a mathematics institute but a materials research institute. This is the director's vision in which AIMR will advance short- and medium-term strategies (partially traditional materials science) first and foremost. At the same time AIMR will expand the scope of its mathematics-materials science collaboration based on a long-term strategy, gradually increasing the degree of penetration of mathematics into materials science, and finally complete the fusion of mathematics and materials science and realize the materials research institute where a touch of mathematics can be found everywhere. In order to advance this challenge more steadily and rigidly, it is necessary for us to evolve the emerging results we have already obtained, and thus a five-year extension is critical for accomplishing our mission.

^{*} Describe the Center's Response to Results of FY2013 Follow-up. Note: If you have already provided this information, please indicate where in the report.

[Suggestion 2]

AIMR was asked to consider possible limitations of the math-mate collaboration and to consider on which area their efforts should be concentrated. That limitations and difficulties may be encountered when pursuing further should be recognized and, therefore, an additional discussion might be necessary on what fields in the materials science should be challenged by the math-mate collaboration.

[Response]

As the Program Committee suggested, the difficulty in mathematics—materials science collaboration depends on the research fields, therefore, which fields should we focus on for collaboration with mathematics should be determined based on thorough discussion. In that case, judgment based on preconceptions or one-sided observations are not appropriate. For example, in the FY2011 Follow-up report by the WPI Program Committee (December 2012), the description "There must be some boundary which cannot simply be resolved by the concept of math-mate collaboration; for example, in some synthetic chemistry," was shown in the section "4. Actions Required and Recommendations." However, afterwards, the synthetic chemistry group (Prof. Hiroyuki Isobe group) succeeded in obtaining an index to give geometric definition to finite carbon nanotubes in collaboration with mathematicians (Pure and Applied Chemistry 86, 489–495 (January 2014)). This suggests that affinity between mathematics and some disciplines is not as difficult as it seems. When we discuss and decide the fields for collaboration with mathematics, we should not omit fields because of preconceptions or one-sided observations, and we must discuss the matter while inclusive of many viewpoints.

[Comment with respect to the efforts toward sustainability]

President Satomi's vision for Tohoku University places AIMR as a role model to reform the entire university. A Task Force was set up and has been drawing plans on the sustainable organizational framework after the end of the WPI Program. It is desirable to make clear how the future new organization is ranked relative to the other existing research centers and how these organizations share the roles in the research on materials science.

[Response]

Tohoku University is strong in materials science and well-known research centers in materials science, such as the Institute for Materials Research (IMR; Kin-ken) and the Institute of Multidisciplinary Research for Advanced Materials (IMRAM; Tagen-ken) already exist. While AIMR is one part of this major foothold of materials science in Japan, AIMR can find its significance of existence by leading Tohoku University in internationalization, system reform, and interdisciplinary fusion research by world-leading researchers and creating new materials science. AIMR will also play an important role as the first institute to be involved in the Organization for Advanced Studies, which will be established in FY2014.

World Premier International Research Center Initiative (WPI) 1. FY 2013 List of Principal Investigators

- NOTE:
 Underline names of investigators who belong to an overseas research institution.
 In case of researchers not listed in the latest report, attach "Biographical Sketch of a New Principal Investigator".

<Results at the end of FY2013>

Principal Investigators Total: 31

	Trincipal investigators	Total. 31							
Name (Age)	Affiliation (Position title, department, organization)	Academic degree, specialty	Working hours (Total working hours: 100%)						Contributions by PIs
			Work on center project		Others		Starting date of project participation	Status of project participation (Describe in concrete terms)	from overseas research
			Research activities	Other activities	Research activities	Other activities	. participation		institutions
Center director Motoko Kotani* (54)	Professor, AIMR, Tohoku University	Dr. of Science, Mathematics (Geometry)	40%	50%	10%	0%	Director: From Apr. 2012 Deputy Director: From May 2011 PI: From Mar. 2011	Usually stays at the center	
Tadafumi Adschiri* (56)	Professor, AIMR, Tohoku University	Dr. of Engineering, Hybrid materials, Super-critical Fluid Technology	80%	0%	0%	20%	From start	Usually stays at the center	
Mingwei Chen* (48)	Professor, AIMR, Tohoku University	Dr. of Engineering, Materials Science	100%	0%	0%	0%	From start	Usually stays at the center	

Masayoshi Esashi* (65)	Professor, AIMR, Tohoku University	Dr. of Engineering Sensors, Micro Electro Mechanical Systems	80%	0%	0%	20%	From start	Usually stays at the center	
Hiroyuki Isobe* (43)	Professor, AIMR, Tohoku University	Ph.D., Organic Chemistry	80%	0%	10%	10%	From Apr. 2013	Usually stays at the center	
Kazue Kurihara* (63)	Professor, AIMR, Tohoku University	Dr. of Physical Chemistry, Colloid and Interface Science	80%	0%	0%	20%	From Apr. 2010	Usually stays at the center	
Dmitri V. Louzguine* (46)	Professor, AIMR, Tohoku University	Dr. of Engineering, Materials Science	100%	0%	0%	0%	Professor: From Dec. 2007 PI: From 2009	Usually stays at the center	
Tomokazu Matsue* (60)	Professor, AIMR, Tohoku University	Dr. of Pharmacy, Biosensing Engineering	80%	0%	0%	20%	From Nov. 2010	Usually stays at the center	
Yasumasa Nishiura* (63)	Professor, AIMR, Tohoku University	Dr. of Science, Applied Mathematics (Nonliner Dynamics)	100%	0%	0%	0%	From Feb. 2012	Usually stays at the center	

Shin-ichi Orimo* (48)	Professor, AIMR, Tohoku University	Ph.D., Materials Engineering and Chemistry	80%	0%	0%	20%	From Jan. 2013	Usually stays at the center	
Eiji Saitoh* (42)	Professor, AIMR, Tohoku University	Dr. of Engineering, Spintronics	80%	0%	0%	20%	From Apr. 2012	Usually stays at the center	
Masatsugu Shimomura* (60)	Professor, AIMR, Tohoku University	Dr. of Engineering, Polymer Science	80%	0%	0%	20%	From start	Usually stays at the center	
Takashi Takahashi* (62)	Professor, AIMR, Tohoku University	Dr. of Science, Solid-State Physics	80%	0%	0%	20%	From start	Usually stays at the center	
Katsumi Tanigaki* (59)	Professor, AIMR, Tohoku University	Dr. of Engineering, Nano Materials Science	80%	0%	0%	20%	From start	Usually stays at the center	
Hideo Ohno∗ (59)	Professor, Research Institute of Electrical Communication, Tohoku University	Dr. of Engineering, Semiconduct or Physics and Engineering, Spintronics	40%	0%	40%	20%	From Apr. 2012	Usually stays at the Institute of Research Institute of Electrical Communication, close to the center, and participate in the center's activities	

Seiji Samukawa* (55)	Professor, Institute of Fluid Science, Tohoku University	Dr. of Nanoprocess Engineering	40%	0%	40%	20%	From Apr. 2012	Usually stays at the Institute of Fluid Science, close to the center, and participate in the center's activities	
Yuichi Ikuhara* (55)	Professor, School of Engineering, University of Tokyo	Dr. of Engineering, Physical Metallurgy	40%	0%	40%	20%	From start	Stays at the center every two weeks	
Benoit Collins* (36)	Associate Professor, Department of Mathematics and Statistics University of Ottawa	Ph.D. Mathematics (Probability Theory)	50%	0%	25%	25%	From Apr. 2013	Stays at the center for about six months in total	Send young scientists to the WPI center (1/2.5 months) (1/2 months) (1/1 month)
Tomasz Dietl* (63)	Professor, Head of Laboratory of Cryogenic and Spintronic Research, Institute of Physics, Polish Academy of Sciences	Dr. Hab., physics of semiconduct ors and magnetic materials, low-tempera ture physics	20%	0%	45%	35%	From Apr. 2012	Stays at the center twice a year Attends the conference	
Thomas Gessner* (59)	Professor, Center for Microtechnologies, Chemnitz University of Technology	Ph.D. in Device Science/ Technology	30%	0%	50%	20%	From start	Stays at the center twice a year Attends the conference Sends young scientists to the center	Send young scientists to the WPI center (1/5.5 years since 2008) (1/1.3 years since 2012) (1/6.5 months) (1/6 months) (1/2.5 months)

Appendix 1

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Alain Lindsay Greer* (58)	Professor, Department of Materials Science & Metallurgy, University of Cambridge	Ph.D. in Metallurgy & Materials Science	20%	0%	45%	35%	From start	Stays at the center twice a year Attends the conference Sends young scientists to the center	Send young scientist to the WPI center (1/1.5 years since 2012)
Kosmas Prassides* (56)	Professor, Department of Chemistry, University of Durham	D.Phil. in Chemistry	20%	0%	45%	35%	From Apr. 2013	Stays at the center every two months Attends the conference Sends young scientists to the center	Send young scientist to the WPI center (1/3 months)
Thomas P. Russell* (61)	Professor, Department of Polymer Science and Technology, University of Masachu- Setts Amherst	Ph.D. in Nano- Science Technology	20%	0%	45%	35%	From start	Stays at the center twice a year Attends the conference	
Alexander Shluger* (59)	Professor, Department of Physics and Astronomy, University College London	Ph.D. in Computation al Materials Science, Condensed Matter Physics	35%	0%	45%	25%	From start	Stays at the center three times (one month in total) a year Attends the conference Sends young scientists to the center	Send young scientists to the WPI center (1/1.6 years since 2012) (1/1 month)
<u>Li-Jun Wan</u> * (56)	Professor, Institute of Chemistry, Chinese Academy of Science	Ph.D. in SPM, Physical Chemistry, Nanoscience and technology	20%	0%	45%	35%	From start	Attends the conference Sends young scientists to the center	Send young scientist to the WPI center (1/6 months)
Paul S. Weiss* (54)	Professor, Department of Chemistry and Biochemistry, University of California, Los Angeles	Ph.D. in Surface Science	20%	0%	45%	35%	From start	Sends young scientists to the center	Send young scientist to the WPI center (1/1.9 years since 2012)

Appendix 1

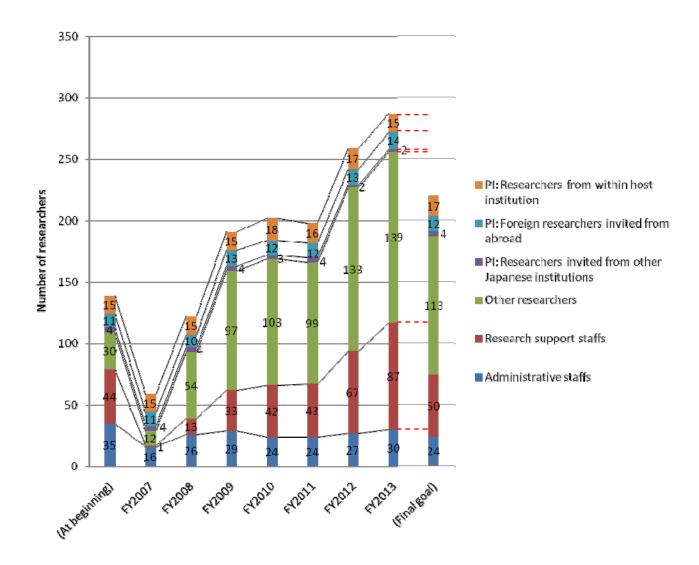
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<u>Qi-kun Xue</u> * (50)	Professor, Department of Physics, Tsinghua University	Ph.D. in Surface Science	20%	0%	45%	35%	From start	Attends the conference Sends young scientists to the center	Send young scientist to the WPI center (1/1.7 years since 2012)
Alain Reza Yavari* (64)	Professor, Grenoble Institute of Technology	Ph.D. in Physical Metallurgry	30%	0%	45%	25%	From start	Stays at the center several times Attends the conference Sends young scientists to the center	Send young scientists to the WPI center (1/5.9 years since 2008) (1/1 month)
Ali Khademhosseini* (38)	Associate Professor, Medical School, Harvard University	Ph.D. in Bioengineeri ng	35%	0%	45%	20%	From Nov. 2009	Stays at the center several times Joins a videoconference regularly from the home institution (Harvard Univ.)	Send young scientists to the WPI center (1/3.9 years since 2010) (1/3 years since 2011) (1/2 years since 2012) (1/5 months Since 2013)
Winfried Teizer* (43)	Associate Professor, Department of Physics, Texas A&M University	Ph.D. in Physics	35%	0%	40%	25%	From Nov. 2009	Stays at the center several times (over three months in total) a year Joins a videoconference regularly from the home institution (Texas A&M Univ.)	Send young scientists to the WPI center (1/3.4 years since 2010)
Hongkai Wu* (35)	Associate Professor, Department of Chemistry, Hong Kong University of Science and Technology	Ph.D. in Chemistry	35%	0%	45%	20%	From Nov. 2009	Stays at the center for a month Joins a videoconference regularly from the home institution (Hong Kong Univ.)	Send young scientists to the WPI center (1/3.5 years since 2010) (1/3.1 years since 2011)

Researchers unable to participate in project in FY 2013

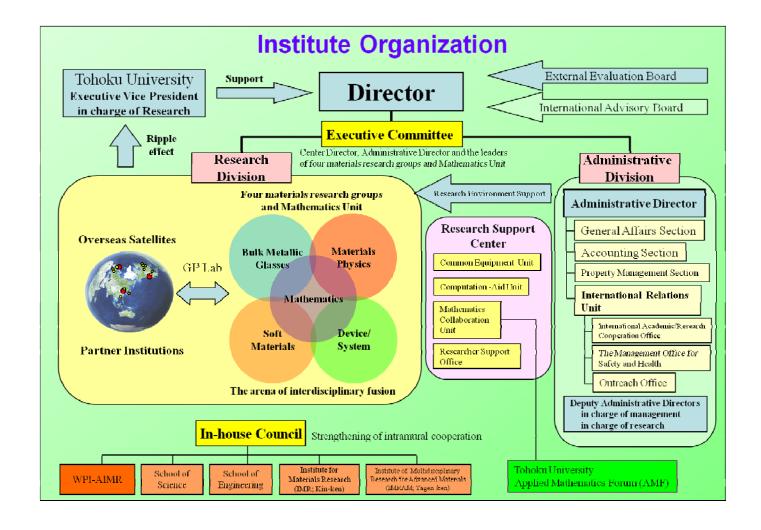
Name	Affiliation (Position title, department, organization)	Starting date of project participation	Reasons	Measures taken
Terunobu Miyazaki	Researcher, AIMR, Tohoku University	From start	Step down from PI because of the age limitation rule of Tohoku University	
Michio Tokuyama	Researcher, Institute of Multidisciplinary Research for Advanced Materials	From start	Step down from PI because of the age limitation rule of Tohoku University	
Kevin J. Hemker	Professor, Department of Mechanical Engineering, Johns Hopkins University	From start	To concentrate on the research at the Johns Hopkins University	

2. Annual transition in the number of Center personnel

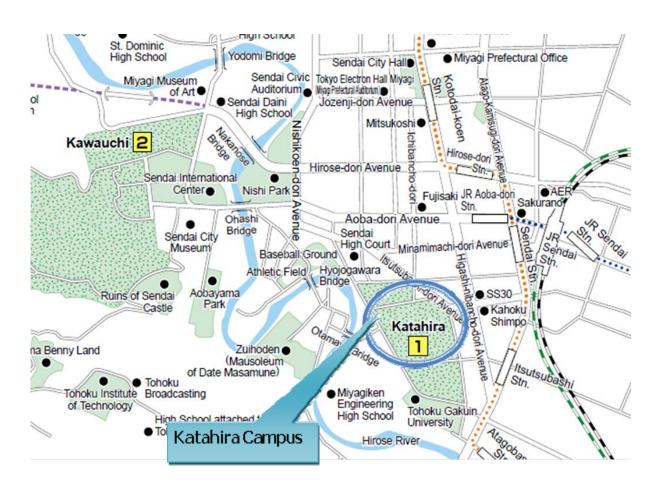
*Make a graph of the annual transition in the number of center personnel since the start of project.



3. Diagram of management system

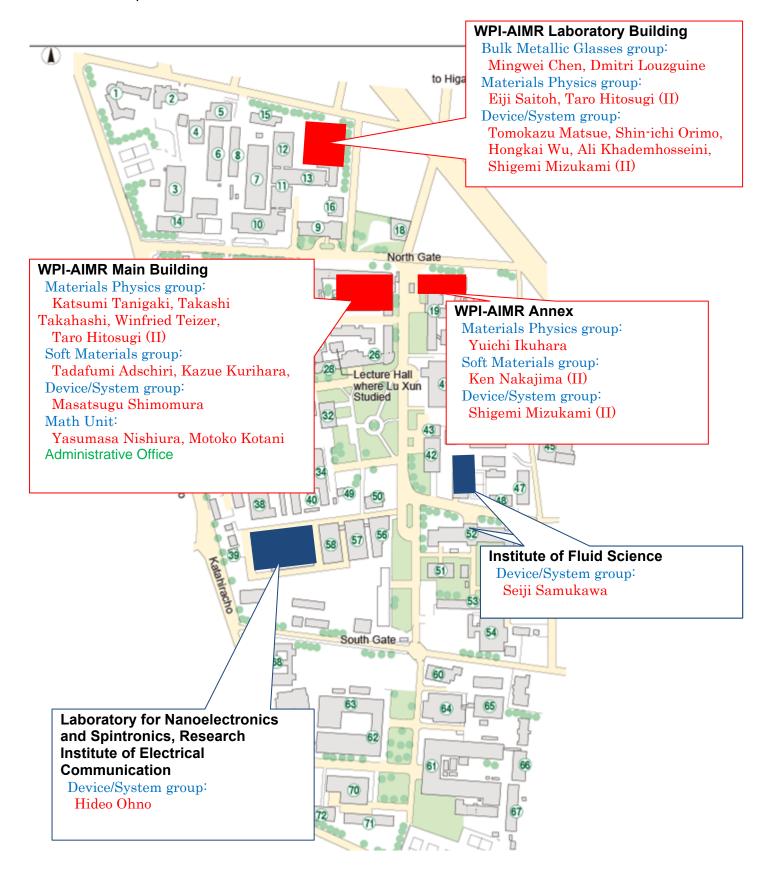


4. Campus map

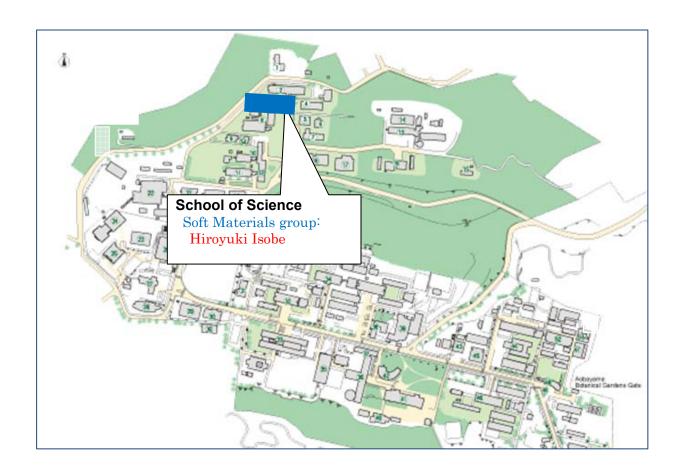




[Katahira Campus]



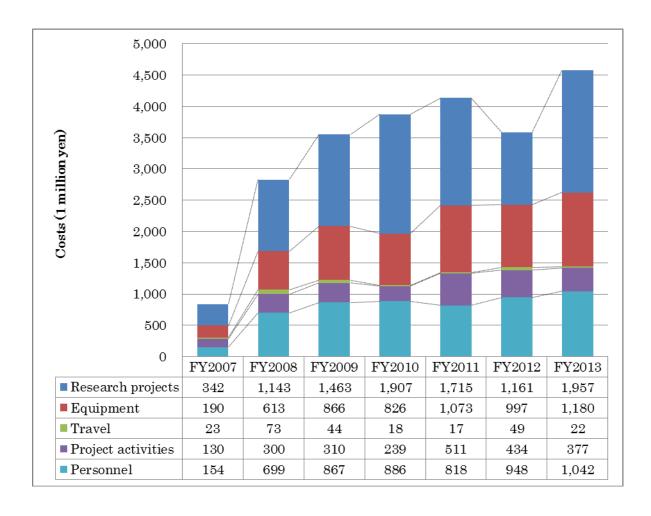
[Aobayama Campus]





5. Annual transition in the amounts of project funding

*Make a graph of the transition in the number of overall project funding.



Ten thousand dollars

Overall project funding

Cost Items	Details	Costs (10,000 dollars)
	Center director and Administrative director	24
	Principal investigators (no. of persons):18	189
Personnel	Other researchers (no. of persons):99	630
	Research support staffs (no. of persons):28	36
	Administrative staffs (no. of persons):41	163
	Total	1042
	Gratuities and honoraria paid to invited principal investigators (no. of persons):11	16
	Cost of dispatching scientists (no. of persons):0	
	Research startup cost (no. of persons):33	116
	Cost of satellite organizations (no. of satellite organizations):3	9
Project activities	Cost of international symposiums (no. of symposiums):1	36
r roject denvines	Rental fees for facilities	
	Cost of consumables	33
	Cost of utilities	65
	Other costs	102
	Total	377
	Domestic travel costs	2
	Overseas travel costs	8
	Travel and accommodations cost for invited scientists	
Travel	(no. of domestic scientists):7	10
	(no. of overseas scientists):14	
	Travel cost for scientists on secondment	
	(no. of domestic scientists):6 (no. of overseas scientists):0	2
	Total	22
	Depreciation of buildings	139
Equipment	Depreciation of equipment	1041
	Total	1180
	Projects supported by other government subsidies, etc.	1100
Other research	Commissioned research projects, etc.	1729
projects	Grants-in-Aid for Scientific Research, etc.	228
•	Total	1957
	Total	4578

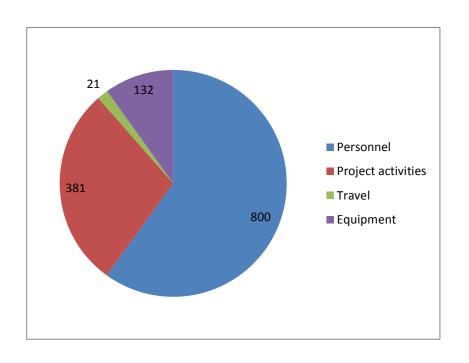
WPI grant	1334
Costs of establishing and maintaining facilities Establishing new facilities (Number of facilities: , m²) Costs paid:	0
Repairing facilities (Number of facilities: , m²) Others Costs paid:	
Cost of equipment procured	1141
Silicon High Aspect Etching Equipment Number of units:1 Costs paid:	99
Integrated Structure Verification System Number of units:1 Costs paid:	92
Nuclear Magnetic Resonance Spectrometer(600MHz) Number of units:1 Costs paid:	80
Single Crystal X-ray System Number of units:1 Costs paid:	57
Environmental Adaptation Verification System Number of units:1 Costs paid:	57
High Resolution Time Of Flight Mass Spectrometry System	55
Multi-purpose X-ray Diffraction System Number of units:1 Costs paid:	52
Device Fabrication System Number of units:1 Costs paid:	49
Physical Properties Measurement Equipment Number of units:1 Costs paid: Spintronics Materials Etching Equipment For Ultra-Small	38
Device	34
Number of units:1 Costs paid: Others	528

ii) Costs of Satellites and Partner institutions

Cost Items	Details	Costs (10,000 dollars)	
	Principal investigators (no. of persons):3		
	Other researchers (no. of persons):15	91	
Personnel	Research support staffs (no. of persons):0	71	
	Administrative staffs (no. of persons):0		
	Total	91	
Project activities		25	
Travel		18	
Equipment			
Other research			
projects			
	Total	134	

i) Overall expenditures

Cost Items	Details	Costs (10,000 dollars)
	Center director and Administrative director	11
	Principal investigators (no. of person):17	53
Personnel	Other researchers (no. of person):102	602
0.00101	Research support staffs (no. of person):29	36
	Administrative staffs (no. of person):31	98
	Total	800
	Gratuities and honoraria paid to invited principal investigators (no. of person):11	16
	Cost of dispatching scientists (no. of person):0	
	Research startup cost (no. of person):33	124
	Cost of satellite organizations (no. of satellite organization):3	9
Project activities	Cost of international symposiums (no. of symposiums):1	36
	Rental fees for facilities	
	Cost of consumables	32
	Cost of utilities	64
	Other costs	100
	Total	381
	Domestic travel costs	1
	Overseas travel costs	8
	Travel and accommodations cost for invited scientists	
Travel	(no. of domestic scientists):7	10
Traver	(no. of overseas scientists):14 Travel cost for scientists on secondment	
	(no. of domestic scientists):6	2
	(no. of overseas scientists):0	_
	Total	21
Equipment	Cost of equipment procured	132
Equipment	Total	132
	Total	1334



ii) Costs of Satellites and Partner institutions

Cost Items	Details	Costs (10,000 dollars)
	Principal investigators (no. of person):3	
	Other researchers (no. of person):15	01
Personnel	Research support staffs (no. of person):0	91
	Administrative staffs (no. of person):0	
	Total	91
Project activities		25
Travel		18
Equipment		
	Total	134

1. List of papers underscoring each research achievement

- * List papers underscoring each research achievement listed in the item 2-1 "Research results to date" (up to 40 papers) and provide a description of the significance of each (within 10 lines).
- * For each, write the author name(s); year of publication; journal name, volume, page(s), and article title. Any listing order may be used as long as format is the same. If a paper has many authors, underline those affiliated with the Center.
- * If a paper has many authors (say, more than 10), all of their names do not need to be listed.
- * Place an asterisk (*) in front of those results that could only have been achieved by a WPI center.

[Observe and understand atoms and molecules]

*Research results 1 Direct observation of atoms on an oxide surface

*1. R. Shimizu, K. Iwaya, T. Ohsawa, S. Shiraki, T. Hasegawa, T. Hashizume and T. Hitosugi, Atomic-scale visualization of initial growth of homoepitaxial SrTiO₃ thin film on atomically ordered substrate. **ACS Nano** 5, 7967-7971 (2011).

Combination of PLD and STM: When an interface of two materials forms, there is a high potential for producing new characteristics; for example, the electric conductivity of the interface of the two insulators lanthanum aluminate and strontium titanate. However, achieving atom scale observation in such interface systems has not happened yet. In this study, the AIMR research group developed a high-resolution scanning tunneling microscope (STM) combined with a pulsed laser deposition (PLD) system, and investigated the homo-epitaxial atom-by-atom growth process of a perovskite material, strontium titanate. They found that the specific surface can be prepared in a wide range of oxygen partial pressures in a reproducible manner. This investigation technique can be applied to the preparation of new heterostructures, or high-quality thin films with remarkable multi-functionality.

*2. <u>K. Iwaya</u>, T. Ogawa, T. Minato, K. Miyoshi, J. Takeuchi, A. Kuwabara, H. Moriwake, Y. Kim, <u>T. Hitosugi</u>, Impact of Lithium-Ion Ordering on Surface Electronic States of LixCoO₂. **Physical Review Letters** 111, 126104 (2013).

Atomic imaging on electrode surfaces: Since Lithium (Li) ions are small and light, they are ideal for carrying a charge between cathodes and anodes in rechargeable batteries, and are thus widely used in commercial lithium-ion batteries. However, the atomic processes behind their movements in battery interfaces have not fully been understood because it has been difficult to observe the interface with an atomic resolution. Recently, researchers from AIMR and their collaborators succeeded in obtaining unprecedented images of atoms on the surface of lithium cobalt oxide (LiCoO₂), used for cathode material in lithium-ion batteries, using scanning tunneling microscopy (STM). They developed the technique to control the Li content in lithium cobalt oxide single crystals and prepared a flat surface for STM observation by cleaving the single crystals in an ultra-high vacuum. The ordered Li atom distribution was observed, and this result is useful for designing high-performance lithium-ion batteries.

*Research results 2 Observation of the arrangement of atoms near grain boundaries

*3. <u>Z.C. Wang</u>, M. Okude, <u>M. Saito</u>, <u>S. Tsukimoto</u>, A. Ohtomo, <u>M. Tsukada</u>, <u>M. Kawasaki</u> and <u>Y. Ikuhara</u>, Dimensionality-driven insulator–metal transition in A-site excess non-stoichiometric perovskites. **Nature Communications** 1, 106 (2010).

Interface and electric conductivity: In this study, a breakthrough method to induce an oxide to become conductive was demonstrated by AIMR researchers. They studied the conductivity of a thin film of a layered oxide composed of lanthanum, strontium, and titanium prepared and atomically controlled using pulsed laser deposition (PLD), finding that SrTiO₃ changes its electronic property from insulating to conductive with an increase in the number of deposited layers. They investigated the effect of inserting the additional insulating layers using a combination of scanning transmission electron microscopy (STEM) and numerical simulations, showing that the addition of the insulating layers reduced distortion and bond strain in the oxide film. Their data show that this conductive behavior arises from the creation of a conductive two-dimensional layer inside the oxide by allowing the material to relax to a less-strained state. The results represent a new method of obtaining electronic materials from insulators.

*4. <u>Z.C. Wang</u>, <u>M. Saito</u>, <u>K.P. McKenna</u>, <u>L. Gu</u>, <u>S. Tsukimoto</u>, <u>A.L. Shluger</u> and <u>Y. Ikuhara</u>, Atom-resolved imaging of ordered defect superstructures at individual grain boundaries. **Nature** 479, 380-383 (2011).

Grain boundary defects: Defects play a crucial role in determining the properties of materials; in particular, grain boundaries essentially influence the properties of polycrystalline materials. The self-trapped grain boundary defect is an especially significant defect, and should be investigated carefully in terms of distribution and role. However, it has been difficult to study such defects systematically, due to their very low concentration. The researchers from AIMR developed a new methodology to elucidate such defects using an artificial "bicrystal," consisting of two crystals cut along different crystallographic directions. The researchers analyzed the sample with a combination of electron energy loss spectroscopy (EELS), transmission electron microscopy measurements, and first-principle calculations using density functional theory (DFT). They discovered that titanium and calcium impurities segregate into grain boundaries. This atomic-scale information on point defects provides insight into quantum level structure-property interplay.

*5. <u>Z.C. Wang</u>, <u>M. Saito</u>, <u>K. P. McKenna</u> and <u>Y. Ikuhara</u>, Polymorphism of dislocation core structures at the atomic scale. **Nature Communications** 5, 3239 (January 2014).

Atomic dislocation core structure: Ceramics have complex crystal structures as compared to metallic materials. Therefore, very small changes in the structure, such as distortions and defects, considerably affect the characteristics of materials; for example, these materials' electric conductivity and thermal conductivity. In other words, such small changes in the structure, such as "dislocations," themselves have great potential to produce novel functions as practical materials. AIMR researchers focused on the dislocations regularly distributed along grain boundaries, and succeeded in complete comparison between simulated dislocation structures predicted by first-principle calculation and artificial dislocations experimentally formed in "bicrystals," consisting of two crystals attached in a variety of offset angles and observed by ultra-high resolution scanning transmission electron microscopy. This leads to the new technique to create dislocation structure which produces novel functions based on theoretical prediction.

resolution "Dirac cone" as the common band dispersion to novel materials

*6. <u>K. Sugawara</u>, T. Sato and <u>T. Takahashi</u>, Fermi-surface-dependent superconducting gap in C₆Ca. **Nature Physics** 5, 40–43 (2009).

Superconductivity in graphite compounds: Superconductivity in some graphite intercalation compounds was discovered over 40 years ago. However, the recently discovered C_6Ca is special, as it remains superconductive to much higher temperatures, as much as 11.5 K. In this study, AIMR researchers investigated this special graphite by angle-resolved photoemission spectroscopy with the world's highest resolution, and obtained an important clue to the origin of the superconductivity. As per the theoretical expectation, an onset of superconductivity by the opening of a gap was observed. However, the gap was seen only for the electronic states of the calcium interlayers, and could not observed for the in-plane states of the graphite sheets. These findings suggest the important role of the interlayer atoms; that is, the calcium atoms "donate" electrons to the graphite layers, and the strong coupling between the calcium electrons and the carbon atoms causes higher superconducting temperature of C_6Ca .

*7. <u>P. Richard</u>, K. Nakayama, T. Sato, M. Neupane, Y.-M. Xu, J.H. Bowen, G.F. Chen, J.L. Luo, N.L. Wang, X. Dai, Z. Fang, H. Ding. and <u>T. Takahashi</u>, Observation of Dirac cone electronic dispersion in BaFe₂As₂. **Physical Review Letters** 104, 137001 (2010).

<u>Dirac cone in iron-based superconductors</u>: AIMR researchers investigated the electronic structure of iron-based superconductor $BaFe_2As_2$, discovered by Japanese researchers in 2008, using angle-resolved photoemission spectroscopy with the world's highest resolution. Surprisingly, they discovered the "Dirac cone" band structure whose existence has been found in graphene or topological insulators, and whose electrons are considered to behave like massless particles. Of course, it is not wholly similar to graphene. While the Dirac cone of graphene is symmetric with respect to momentum, the cone for $BaFe_2As_2$ is distinctly asymmetric and displays small pocket-like features and nodes. Although such special features are subject to further research, it is clear that this special band structure is the key to solving the mystery of why these kinds of iron-based magnetic compounds can become superconductors.

8. T. Sato, K. Segawa, K. Kosaka, <u>S. Souma</u>, K. Nakayama, K. Eto, T. Minami, Y. Ando and <u>T. Takahashi</u>, Unexpected mass acquisition of Dirac fermions at the quantum phase transition of a topological insulator. **Nature Physics** 7, 840-844 (2011).

Topological insulator with electrons no longer massless: Topological insulators are among the most promising materials for next-generation electronics. One of the most characteristic features of topological insulators is that electrons at the surface behave as particles with no mass (Dirac fermions). However, in this study, AIMR researchers discovered that electrons do have mass in some topological insulators. They used an angle-resolved photoemission spectrometer (ARPES) with the world's highest resolution, which they developed. They measured the topological insulator, thallium–bismuth–selenium, and compared it with samples where selenium was partially replaced by sulfur. By increasing the sulfur content toward the thallium–bismuth–sulfur composition (not a topological insulator), the "X"-shaped energy dispersion gradually fell and a gap opened up, indicating that the electrons were no longer massless. This discovery suggests new possibilities for applications of topological insulators in information storage.

*9. <u>Y. Tanaka</u>, Z. Ren, T. Sato, K. Nakayama, <u>S. Souma</u>, <u>T. Takahashi</u>, K. Segawa and Y. Ando, Experimental realization of a topological crystalline insulator in SnTe. **Nature Physics** 8, 800–803 (2012).

Topological insulators occurring from both time-reversal symmetry and crystal symmetry: Topology is a concept of the fundamental relationships between the properties of geometrically different objects. Most recently, in solid state physics, attention has been focused upon the interesting properties of topological insulators which consist of an insulating bulk with conductive surfaces. This unique topological property arises from the time-reversal symmetry of a material's electronic states. In this study, AIMR researchers discovered, by means of high-resolution angle-resolved photoemission spectroscopy, an interesting class of crystalline tin telluride-based topological insulators whose properties arise from a combination of both time-reversal and crystal symmetry. This discovery marks a new way of finding topological insulators, and provides significant implications for the development of innovative electronic devices.

*Research results 4 Mapping the mechanical characteristics of polymers with AFM

*10. <u>D. Wang</u>, <u>S. Fujinami</u>, <u>K. Nakajima</u> and <u>T. Nishi</u>, True surface topography and nanomechanical measurements on block copolymers with atomic force microscopy. **Macromolecules** 43, 3169–3172 (2010).

Nanoscale mechanical mapping: Detailed measurements on the phase separation of block copolymers were conducted using atomic force microscopy (AFM). Transmission electron microscopy (TEM) has conventionally been used for this type of research, which provides only structural images, but also has a significant drawback in that the electron beam damages the specimen. Early attempts with AFM also had a serious problem in that the microprobe deformed the polymer. However, with technological developments in compensating for the distortion of the cantilever and displacement of the sample scanner, it is now possible to obtain the mechanical characteristics, including adhesiveness and stiffness, (Young's modulus) in a micro area, as well as structural data. It has become clear that this new technique can be applied to the nano-scale mechanical property mapping of biomaterials, which could not be measured using conventional AFM because they are too soft and fragile to stimulus by cantilever.

*Research results 5 Elucidation of atomic structures in metallic glasses

*11. <u>T. Fujita</u>, K. Konno, W. Zhang, V. Kumar, M. Matsuura, A. Inoue, <u>T. Sakurai</u> and <u>M.W. Chen</u>, Atomic-scale heterogeneity of a multicomponent bulk metallic glass with excellent glass forming ability. **Physical Review Letters** 103, 075502 (2009).

Atomic-scale heterogeneity makes a better metallic glass: The technique to create bulk metallic glasses (BMGs) has been studied for many years. Previous studies revealed its empirical rules; for instance, certain combinations of metals tend to prevent crystallization and enhance the feasibility of producing BMGs. However, it remains unclear exactly why these combinations can form BMGs easier than others. In this study, the atomic arrangement of silver-bearing copper-zirconium BMG was investigated using extended X-ray absorption fine structure (EXAFS) spectroscopy of SPring-8 in order to elucidate the process of the dramatic increase in glass-forming performance of this silver-bearing BMG system. The investigation revealed that there were two types of structures: a shell-like cluster that was rich in zirconium to which silver was connected, and a cluster that was rich in copper as a whole. It also suggested that this atomic-scale un-uniformity was effective for improving glass-formation performance.

*12. <u>A. Hirata, P. Guan, T. Fujita, Y. Hirotsu, A. Inoue, A. R. Yavari, T. Sakurai</u> and <u>M.W. Chen, Direct observation of local atomic order in a metallic glass. **Nature Materials** 10, 28-33 (2011).</u>

<u>Discovery of a short-range order and clusters in BMG</u>: Although various atomic models for metallic glasses exist, none of them has been confirmed because we have been able to obtain only average data over relatively large volumes. In this study, AIMR researchers observed the Zr-Ni-based BMG with a scanning transmission electron microscope (STEM), and succeeded in obtaining electron diffraction patterns from atomic clusters with narrow electron beams. By correcting for spherical aberrations in their electron optics and using a specially designed electron beam condenser aperture, they were able to reduce the diameter of their electron beam to about 0.3 nanometers, the narrowest coherent electron beam demonstrated so far. This much narrower beam produced a distinct set of diffraction spots that could only result from a single crystal, confirming predictions that metallic glasses are composed of small ordered atomic clusters as fundamental structural units, even though these materials are disordered on larger scales.

*13. <u>A. Hirata, T. Fujita, Y.R. Wen, J.H. Schneibel, C.T. Liu</u> and <u>M.W. Chen, Atomic structure of nanoclusters in oxide-dispersion-strengthened steels. **Nature Materials** 10, 922-926 (2011).</u>

Nanoclusters in high strength steels: Using the latest microscopy technology, Cs-corrected scanning transmission electron microscopy (STEM) with a resolution of about 0.1 nanometers, the atomic structures of oxide nanoclusters less than 4 nanometers in size were found in oxide-dispersion-strengthened (ODS) steel. Although an imaging of the cluster has not yet been achieved so far, owing to the effects of the magnetic steel matrix, the atomic structure of the nanoclusters has clearly been identified by minimizing the magnetic effects through the preparation of ultrathin samples about 5 nanometers thick. The surprising result is that the nanoclusters have unusually defective rock salt crystal (NaCl-type) structures, yet are incredibly stable at high temperatures. This is the key to solving the mystery of why ODS shows outstanding resistance to radiation damage and high temperatures.

*14. <u>A. Hirata</u>, <u>L. J. Kang</u>, <u>T. Fujita</u>, B. Klumov, K. Matsue, <u>M. Kotani</u>, <u>A. R. Yavari</u>, <u>M. W. Chen</u>: Geometric frustration of icosahedrons in metallic glasses. **Science** 341, 376-379 (2013). (This paper overlaps with the interdisciplinary research result shown in Appendix 3.)

Mathematics-materials science collaboration: The fusion research team of mathematicians and experimentalists at AIMR successfully characterized the atomic structure in metallic glass and revealed atomic-scale competition in energy and geometry for glass formation. The experimentalists developed an angstrom beam electron diffraction method, analyzing the local atomic structure. Mathematicians applied "computational homology" to analyze the observed structure. This collaboration unveiled the long-standing mystery of atomic configurations: that geometric distortions of icosahedral clusters in metallic glass can be scaled up to long-range disorder in a simple manner with topological connectivity. The co-existence of icosahedral and FCC-crystal-like symmetries in the distorted icosahedral clusters leads to the perfect distortion for making a disordered, densely-packed structure. The underlying discrepancy that remained unknown for half a century has been solved.

[Control atoms and molecules]

*Research results 6 Oxide electronics: superconductivity and fractional quantum Hall effect

*15. <u>K. Ueno</u>, S. Nakamura, H. Shimotani, A. Ohtomo, N. Kimura, T. Nojima, H. Aoki, Y. Iwasa and <u>M. Kawasaki</u>, Electric-field-induced superconductivity in an insulator. **Nature Materials** 7, 855–858 (2008).

Manifestation of Superconductivity by Field-Effect Doping 1: Strontium titanate (SrTiO₃) is an insulator that does not normally conduct current. However, its superconductivity was realized by injecting a large amount of electrons onto the surface of SrTiO₃ by "field-effect doping," which forms an electric double layer on the sample's surface by applying gate voltage to an electrolyte solution. Conventional attempts include impurity doping, which involves charge injection using a chemical method. This research has achieved a superconducting transition by field-effect doping, for the first time in history. The realization of superconductivity in a clean method without using impurities has made a significant impact, both in terms of basics and applications.

*16. <u>K. Ueno</u>, S. Nakamura, H. Shimotani, H.T. Yuan, N. Kimura, T. Nojima, H. Aoki, Y. Iwasa and <u>M. Kawasaki</u>, Discovery of superconductivity in KTaO₃ by electrostatic carrier doping. **Nature**Nanotechnology 6, 408–412 (2011).

Manifestation of Superconductivity by Field-Effect Doping 2: AIMR, in collaboration with researchers from the University of Tokyo, have succeeded in producing a superconducting state by artificially introducing large amounts of electrical charges into known materials, such as potassium tantalum oxide (KTaO₃). They created an electric double layer transistor structure using ionic liquid. By bringing the ionic liquid into contact with the surface of an electrical circuit containing the material, an electric double layer is formed at the material–liquid interface. By applying an electrical voltage to the gate electrode, a large amount of carriers are doped into the material due to the large electric field in the electric double layer, compared to general field effect transistors (FETs). Since this method does not face the same limitations as chemical doping, this approach has great potential to realize superconductor systems even for materials that have not shown superconductivity through chemical doping.

17. A. Tsukazaki, S. Akasaka, K. Nakahara, Y. Ohno, <u>H. Ohno, D. Maryenko</u>, A. Ohtomo and M. <u>Kawasaki</u>, Observation of the fractional quantum Hall effect in an oxide. **Nature Materials** 9, 889–893 (2010).

<u>Fractional Quantum Hall Effect in an Oxide Material</u>: A fractional quantum Hall effect in an oxide material was confirmed for the first time ever by depositing a magnesium oxide zinc thin film on zinc oxide through atomic-level control. An extremely thin and smooth interface is required to realize a quantum transport phenomenon in which two-dimensional electrons move freely, according to quantum mechanics. However, it has been difficult to actualize quantum transport phenomena in oxide-based materials which tend to contain impurities and defects. Based on a long experience of controlling oxides on the atomic level, the researchers succeeded in suppressing electron scattering by using their technology to create a high quality oxide interface (with electron mobility six times higher than usual) comparable to some leading-edge semiconductors, and in observing the fractional quantum Hall effect. This result suggests the possibility of the future application of oxide materials, such as zinc oxide, to quantum calculations.

*18. <u>A. Kumatani, T. Ohsawa, R. Shimizu, Y. Takagi, S. Shiraki, and T. Hitosugi, Growth processes of lithium titanate thin films deposited by using pulsed laser deposition. **Applied Physics Letters** 101, 123103 (2012).</u>

<u>Transparent superconductors by stoichiometry control</u>: Composite oxides exhibit intriguing physical properties, such as superconductivity and magnetism, and have been applied to various devices such as transistors and batteries. In order to improve the performance of these materials, control of the

stoichiometry (atomic ratio of the elements in chemical formulae) is an essential requirement. AIMR researchers studied the growth of lithium titanate oxides (spinel) and succeeded in creating transparent superconducting thin films through precise control of the stoichiometry. They first focused on $\text{Li}_4\text{Ti}_5\text{O}_{12}$, commonly used as an electrode in lithium-ion batteries, and found that they could obtain LiTi_2O_4 thin films with low oxygen partial pressure during pulsed laser deposition (PLD). These thin films exhibited transmittance of visible light of up to 70%, as well as a critical temperature for superconductivity of 13 K, a world record for such a transparent thin film.

*Research results 7 Spintronics : Controlling "spin"

*19 <u>L. Chen, F. Matsukura</u>, and <u>H. Ohno</u>, Direct-current voltages in (Ga,Mn)As structures induced by ferromagnetic resonance. **Nature Communications** 4, 2055 (2013).

Establishment of quantitative analysis technique for spin current: Spin currents can be used in spintronics, while only charge currents (flow of electrons) are used in conventional electronics. A pure spin current is converted to a charge current by the spin-orbit interaction, and produces a measureable DC voltage via the inverse spin Hall effect. Although the spin current can be estimated by measuring this voltage, the value includes other current/voltage components which do not originate from spin current; for example, a component from ferromagnetic resonance through galvanomagnetic effects. Therefore, a technique to distinguish these is necessary. In this study, AIMR researchers investigated the (Ga,Mn)As/p-GaAs layered structure as a model system, and found that the measured voltage can be separated into components which originated from spin current and others. This technique is expected to contribute to fundamental and applied studies of spin currents.

20. T. An, V. I. Vasyuchka, K. Uchida, A. V. Chumak, K. Yamaguchi, K. Harii, J. Ohe, M. B. Jungfleisch, Y. Kajiwara, H. Adachi, B. Hillebrands, S. Maekawa, and <u>E. Saitoh</u>, "Unidirectional spin-wave heat conveyer" **Nature Materials** 12, 549–553 (2013).

Heat energy conveyance using magnetic waves: In general, charge currents or microwave are used for inputting and outputting information into/from devices. However, in this case, a lot of energy is consumed for heat generation, and furthermore, the heat makes devices unstable. Thus, an effective technique to discharge the heat is sought after. In this study, AIMR researchers and their collaborators discovered the basic principle for heat energy conveyance to desired direction using the magnetic waves (spin waves) and succeeded in confirming this principle by experiments using ferrimagnetic $Y_3Fe_5O_{12}$. They demonstrated the controllable heat flow caused by a spin-wave current, and also showed that the direction of the flow can be switched by applying a magnetic field. This finding will contribute to the development of next-generation energy-saving device technology.

*21. <u>A. Takayama</u>, T. Sato, <u>S. Souma</u>, T. Oguchi and <u>T. Takahashi</u>, Tunable spin polarization in bismuth ultrathin film on Si(111). **Nano Letters** 12, 1776–1779 (2012).

Spin polarization due to Rashba effect and changing the film thickness: Ferromagnetic materials, in which spins are naturally aligned, have been used for producing spin-polarized electrons. However, for device applications, electric fields are often preferred to magnetic ones. In that case, "spin-orbit coupling," which connects the charge of an electron with its spin for spin polarization, is used. The "Rashba effect" is one of the typical examples for achieving that. AIMR researchers have studied the Rashba effect in very thin films of the metal bismuth. They deposited films of thickness ranging from 16 to 80 atomic layers on a

silicon surface, observing that the spin-polarizing effect was at work not only on the surface, but also at the interface between the metal film and the silicon substrate. They also showed that the degree of polarization is tunable through the thickness of the films. These materials hold great promise for applications in next-generation spintronics devices and for fundamental studies of novel quantum effects.

*22. <u>T. Arakane</u>, T. Sato, <u>S. Souma</u>, K. Kosaka, K. Nakayama, M. Komatsu, <u>T. Takahashi</u>, Z. Ren, K. Segawa and Y. Ando, Tunable Dirac cone in the topological insulator Bi_{2-x}Sb_xTe_{3-y}Se_y. **Nature Communications** 3, 636 (2012).

Controlling the current leakage from surface to bulk in topological insulators: In ideal topological insulators, the bulk volume does not pass any currents although their surface is highly conductive. However, the bulk of an existing topological insulator often has defects through which currents can flow. This bulk current can obscure surface currents whose behavior is the intended subject of the experiment. By using BSTS, a material made from bismuth, antimony, tellurium, and selenium for a measurement sample, AIMR researchers showed that manipulating the composition of a topological insulator can keep its bulk conductivity low while also allowing the surface current to be tuned between positive and negative charge carriers. They also revealed that this compositional control can also be used to adjust the energy of the surface charge carriers through angle-resolved photoemission spectroscopy (ARPES). This research will lead to observing a variety of exotic quantum effects.

*Research results 8 Phonon engineering: Controlling "lattice vibration"

*23. <u>J. Tang</u>, <u>J. Xu</u>, <u>S. Heguri</u>, H. Fukuoka, S. Yamanaka, K. Akai and <u>K. Tanigaki</u>, Electron–phonon interactions of Si₁₀₀ and Ge₁₀₀ superconductors with Ba atoms inside. **Physical Review Letters** 105, 176402 (2010).

Control of phonons by "rattling": New phonon engineering based on atomic vibration in a cage-type structure has suggested a method providing for high \mathcal{T}_c superconductivity. This research used a unique substance including barium as guest atoms in a cage-type structure consisting of a silicon or germanium network, and investigated in detail the relationship between the free motion of barium atoms inside the cage (so-called anharmonic rattling phonons) and physical properties. More specifically, two types of clathrates were compared, $Ba_{24}Si_{100}$ and $Ba_{24}Ge_{100}$, where it was found that substances with large cages and hence strong electron-lattice interactions have unexpectedly inferior superconductivity characteristics. This suggests the possibility of creating new superconductors by devising the design of the cage-type structure. Expectations for new thermoelectric conversion using electron-lattice interactions are also discussed.

*Research results 9 Dynamics between two surfaces and solid/liquid interface

*24. <u>F. Federici Canova</u>, H. Matsubara, M. Mizukami, <u>K. Kurihara</u> and <u>A. L. Shluger</u>, Shear Dynamics of Nanoconfined Ionic Liquids. **Physical Chemistry Chemical Physics** 16, 8247-8256 (February 2014).

<u>Observation of interface dynamics</u>: The relationship between molecular level structure and shear dynamics of the contact interface of ionic liquids was studied using molecular dynamics simulation technique. The researchers used two kinds of ionic liquids [BMIM][NTF2] and [BMIM][BF4] whose cation is the same

1-butyl-3-methyl-imidazolium [BMIM], while anions are different; the former consists of bis(trifluoromethanesulphonyl)amide [NTF2] and the latter consists of tetrafluoroborate [BF4]. They investigated the configuration situation where such ionic liquids are sandwiched between two hydroxylated silica surfaces. The molecular dynamics calculation revealed how the shape of ionic liquids molecules affects their layering structure at hydroxylated silica surfaces, and how the layered structure of nanoconfined liquids determines their dynamical properties at the molecular level. This result qualitatively explains the experimental result of viscosity change of confined ionic liquids.

*Research results 10 Controlling polymerization

*25. L. Dou, <u>Y. Zheng</u>, X. Shen, G. Wu, K. Fields, W.-C. Hsu, H. Zhou, Y. Yang, and <u>F. Wudl</u>, Single-crystal linear polymers through visible light-triggered topochemical quantitative polymerization. **Science** 343, 272–277 (2014).

<u>Creating polymer single crystals</u>: Single crystals of polymers can be difficult to obtain because their long and flexible backbones tend to get tangled, forming structures with no long-range order. However, it can be possible if polymerization takes place inside a molecular crystal in which the reactive monomers are pre-organized in a position that almost corresponds with the repeat distance of the desired polymer. In this study, researchers from the AIMR joint laboratory at University of California, Santa Barbara have used this approach to synthesize a new class of polymers, succeeding for the first time in constructing polymer single crystals from bis(indenedione) monomers by irradiation of "visible light." This polymerization occurs also in concentrated solutions and semicrystalline thin film. Also, the polymers can be decomposed into monomers by heat. Color changes occur due to polymerization and decomposition, thus the progress of the reaction can be seen with the naked eye. These benefits will lead to various applications.

[Create new materials]

*Research results 11 Metallic glass nanowire

*26. <u>K.S. Nakayama</u>, <u>Y. Yokoyama</u>, T. Ono, <u>M.W. Chen</u>, K. Akiyama, <u>T. Sakurai</u> and A. Inoue, Controlled formation and mechanical characterization of metallic glassy nanowires. **Advanced Materials** 22, 872–875 (2010). (This paper overlaps with the interdisciplinary research result shown in Appendix 3.)

Ideal nanowires without grain boundaries: This paper showed the capability of metallic glasses for creating nanowires and their useful application. As opposed to crystalline nanomaterials, metallic glasses have no defects or grain boundaries. When it is heated above the glass transition temperature, its viscosity suddenly drops, enabling super-plastic deformation which enables the creation of long nanowires by extension. The lack of grain boundaries also helps the long extension of the wire. AIMR researchers succeeded in creating metallic glass nanowires of less than 40 nm in diameter by exploiting this property. In collaboration with the micro electro mechanical systems (MEMS) laboratory, they have succeeded in derivation of Young's modulus with the resonant measurement of the metallic glass nanowires, thus opening up possibilities for application to nanoresonators.

Research results 12 Organic/inorganic hybrid nanocrystals

27. J. Zhang, H. Kumagai, K. Yamamura, S. Ohara, S. Takami, A. Morikawa, H. Shinjoh, K. Kaneko, <u>T. Adschiri</u> and A. Suda, Extra-low-temperature oxygen storage capacity of CeO₂ nanocrystals with cubic facets. **Nano Letters** 11, 361–364 (2011).

"Nanocubes" as highly efficient catalysts: Generally, three-way catalysts containing cerium oxide (CeO₂) are widely used in automobiles' exhaust systems. It has been known that control of not only the crystal structure and size, but also the exposed crystal planes, is important for obtaining higher efficiency as catalysts. However, it has been thought impossible to bare the catalytically active planes because they are unstable. In this study, AIMR researchers succeeded in producing CeO₂ "nanocubes" surrounded by the most catalytically active (100) plane. They stopped the plane's growth by capping the surface with organic molecules under supercritical hydrothermal conditions in which organic and inorganic materials could be combined. Measurement of the oxygen storage capacity (OSC: an indicator of catalytic activity) revealed that such nanocubes have a large OSC at much lower temperatures (150 °C) than ordinary CeO₂ catalysts, suggesting that (100)-exposed CeO₂ nanocubes have much higher catalytic activity.

*Research results 13 Nanoporous metals for highly efficient catalysts and supercapacitors

*28. N. Asao, Y. Ishikawa, N. Hatakeyama, Menggenbateer, Y. Yamamoto, M. Chen, W. Zhang and A. Inoue, Nanostructured materials as catalysts: Nanoporous-gold-catalyzed oxidation of organosilanes with water.

Angewandte Chemie International Edition 49, 10093–10095 (2010). (This paper overlaps with the interdisciplinary research result shown in Appendix 3.)

Nanoporous metals as highly efficient catalysts: It is becoming clear that nanoporous metals created through electrochemical treatment (dealloying treatment) function as highly-efficient catalysts. This research used nanoporous gold obtained by selectively dissolving the silver part of a gold-silver alloy, revealing that the oxidation reaction of organic silane compounds was promoted at room temperature, and that the catalyst can be reused multiple times without degrading its catalytic properties. Conventional attempts have created gold nanoparticles supported on a substrate. However, these particles have a short lifespan owing to agglomeration, and the recovery process was cumbersome. There are great expectations for our nanoporous metallic catalyst in future applications.

*29. <u>X. Lang</u>, <u>A. Hirata</u>, <u>T. Fujita</u> and <u>M.W. Chen</u>, Nanoporous metal/oxide hybrid electrodes for electrochemical supercapacitors. **Nature Nanotechnonogy** 6, 232-236 (2011).

Nanoporous metals as large capacity supercapacitors: As a technique for energy storage for society in the future, the importance of double-layer supercapacitors will increase. A team at AIMR has been working on building supercapacitors using transition metal compounds such as manganese dioxide (MnO₂), which can store charges at metal sites through an electron transfer process called 'pseudocapacitance.' The problem is that MnO₂ has low conductivity, which limits charging and discharging speeds. The researchers solved this problem by making a supercapacitor constructed using an MnO₂-plated gold film. First, they selectively etched a silver–gold alloy into a thin gold sheet permeated with numerous nanopores. They then grew MnO₂ nanocrystals directly into the pore channels using a gas-phase reaction. The supercapacitor device displayed excellent charge storage capacity with an energy density up to 20 times higher than that of other MnO₂ electrodes.

*Research results 14 Ultra-hard ceramics

*30. <u>K. M. Reddy</u>, <u>J. J. Guo</u>, Y. Shinoda, <u>T. Fujita</u>, <u>A. Hirata</u>, J. P. Singh, J. W. McCauley and <u>M. W. Chen</u>, Enhanced mechanical properties of nanocrystalline boron carbide by nanoporosity and interface phases. **Nature Communications** 3, 1052 (2012).

New idea for strengthening ceramics: Despite being hard enough to repel bullets, boron carbide ceramics suffer from a critical brittleness that causes them to fracture at low stress levels. This is because ceramics are commonly made by sintering at a temperature just below their melting point, which also generates a variety of crystal grain structures that may act as fracture initiation points. However, AIMR researchers discovered a way to enhance the durability of boron carbide by synthesizing it into a 'nanocrystalline' ceramic with plastic deformation capabilities. They lowered the sintering temperature and used intense pressures to form the boron carbide crystallites with uniform grain sizes, with the expectation that this would reduce brittleness. In addition, they found that tiny, irregularly-shaped nanopores, as well as thin amorphous carbon layers, coated the crystal and nanopore surfaces. These helped to lubricate the crystal grains, enabling them to slide during compression and therefore tolerate greater pressures.

*Research results 15 Biomaterials

*31. <u>J. Ramón-Azcón</u>, <u>S. Ahadian</u>, R. Obregón, G. Camci-Unal, <u>S. Ostrovidov</u>, V. Hosseini, H. Kaji, K. Ino, <u>H. Shiku</u>, <u>A. Khademhosseini</u> and <u>T. Matsue</u>, Gelatin methacrylate as a promising hydrogel for 3D microscale organization and proliferation of dielectrophoretically patterned cells. **Lab on a Chip** 12, 2959–2969 (2012).

A scaffold for longer-lasting cells: Natural tissues are highly organized structures, often formed from multiple cell types precisely positioned to carry out their required roles. Although efforts to mimic these structures in order to create artificial tissues—for example, to help heal body parts that have sustained damage from injury or disease have been conducted—this is no simple task. AIMR researchers developed a highly biocompatible scaffold material that could solve this problem. They selected a semi-natural hydrogel material gelatin methacrylate (GelMA) and first confirmed that it was a suitable matrix within which to guide cells into an appropriate position using dielectrophoresis. Once the cells were in place, the researchers exposed the scaffold to UV light. This triggers a chemical cross-linking reaction within the hydrogel, which forms the polymer matrix and traps the cells in place. Crucially, the cells retain long-term viability after the formation of the cross-linked polymer, and readily proliferate over several days.

*32. <u>T. Fujie</u>, Y. Mori, S. Ito, M. Nishizawa, H. Bae, N. Nagai, H. Onami, T. Abe, <u>A. Khademhosseini</u>, and H Kaji, Micropatterned polymeric nanosheets for local delivery of an engineered epithelial monolayer. **Advanced Materials** 26, 1699-1705 (March 2014).

<u>Ultrathin polymer-based "nanosheets"</u>: Tissue engineering is expected to offer innovative regenerative approaches for cell organization and delivery in the body. AIMR researchers developed ultrathin polymer "nanosheets" that support cell growth and transplantation in a specific location. In order to manufacture the nanosheets, the researchers deposited the biodegradable polymer poly(lactic-co-glycolic) acid, together with magnetic nanoparticles to aid manipulation of the nanosheets, on a microscopic stamp. The researchers then transferred the micropatterned layer onto a glass surface pre-coated with a sacrificial

polymer that, when dissolved in water, releases the nanosheet from the surface. They succeeded in creating the desired "nanosheets" in this way, and obtained some favorable results when they carried out some tests for medical applications.

[Create new devices and systems]

Research results 16 Energy materials and devices

33. W. Hu, M. Igarashi, M.-Y. Lee, <u>Y.M. Li</u> and <u>S. Samukawa</u>, Realistic quantum design of silicon quantum dot intermediate band solar cells. **Nanotechnology** 24, 265401(2013).

Quantum dots for improving solar cells: There exists a theoretical limit, called the Shockley–Queisser (S–Q) limit, in the Si-based solar cell efficiency. The quantum dot (QD) solar cell is a promising candidate to break the (S–Q) limit. The well-aligned QD superlattice is expected to form minibands between the valence band and the conduction band, which induces an extra two-photon-transition from the valence band to the conduction band via the intermediate band. In this study, a highly-periodical Si nanodisk superlattice was fabricated by our top-down process, and the solar cell efficiency of such a structure was evaluated by both experimental study and theoretical simulations. Both the experiments and simulations revealed that miniband formation enhances the optical and electrical collections. Furthermore, theoretical calculation predicted that there is the optimal Si nanodisk superlattice structure which could realize the maximal efficiency of 50.3%.

34. R. Sato, H. Saitoh, N. Endo, S. Takagi, M. Matsuo, K. Aoki, and <u>S. Orimo</u>, Formation process of perovskite-type hydride LiNiH₃: In situ synchrotron radiation X-ray diffraction study. **Applied Physics Letters** 102, 091901 (2013).

Complex hydrides for energy conversion, storage, and transport: ABX₃ perovskites have attracted considerable attention, owing to their specific structure and resulting electronic structure. In this study, AIMR researchers focused on the perovskite-type hydride LiNiH₃, and succeeded in elucidating their formation process using *in situ* synchrotron X-ray diffraction measurements at SPring-8 for the first time ever. A mixture of LiH and Ni was hydrogenated at 873 K and 3 GPa. Time-resolved X-ray diffraction profiles revealed a three-step reaction: first was hydrogenation of Ni to NiH_x, next the formation of Li_yNi_{1-y}H solid solution, and finally the conversion to perovskite-type hydride LiNiH₃. In particular, the discovery that the solid solution Li_yNi_{1-y}H plays the role of the precursor in the perovskite formation is a great step forward for future applications.

*Research results 17 Memory device using tunnel magnetoresistance (TMR)

*35. <u>S. Mizukami</u>, F. Wu, A. Sakuma, J. Walowski, D. Watanabe, <u>T. Kubota</u>, X. Zhang, H. Naganuma, M. Oogane, Y. Ando and <u>T. Miyazaki</u>, Long-lived ultrafast spin precession observed in manganese alloys films with a large perpendicular magnetic anisotropy. **Physical Review Letters** 106, 117201 (2011).

Mn-Ga alloy for TMR devices: Magnetic materials continue to be used as storage systems for computers, and smaller bit sizes are required to increase storage densities. However, as bits become smaller, the

long-term stability of the stored data begins to suffer. AIMR researchers discovered that an alloy of manganese and gallium is not only a strong magnet, but also has switchable magnetization with low loss, which is a key requirement for producing fast, low-power non-volatile magnetic memory. In this study, magnetic friction was measured with an ultrashort laser pulse. The slowdown of the precession after a given amount of time can be probed by a second laser pulse, which allows the magnetic friction coefficient to be calculated. In this study, the researchers found the magnetic friction to be surprisingly low in manganese–gallium alloys. Theoretical calculations indicated that this reduced friction is caused by a very low density of available electronic states at the topmost electron energies in the material.

*36. <u>X. Zhang</u>, <u>S. Mizukami</u>, <u>T. Kubota</u>, <u>Q. Ma</u>, M. Oogane, H. Naganuma, Y. Ando, and <u>T. Miyazaki</u>, Observation of a large spin-dependent transport length in organic spin valves at room temperature. **Nature Communications** 4, 1392 (2013).

Organic spintronics: Research efforts have so far focused on solid-state inorganic materials that can be fabricated to high purity, easily incorporated into devices, and whose composition can be precisely controlled. However, since organic materials are typically made from light elements, mainly from carbon, the spin-orbit interaction is quite small. This means that the electron spin can be preserved for a long time and electrons can, in principle, travel long distances without flipping their spin. In this study, AIMR researchers have realized devices based on organic materials in which electrons can travel long distances at room temperature while preserving their spin. The researchers constructed spin valve devices using fullerene (C_{60}) films with various thicknesses, and observed the very long distance travelling up to 110 nanometers for magnetoresistance at room temperature. This result opens new insights into spintronics.

*Research results 18 Biomimetics: hierarchical structures and functions

*37. <u>D. Ishii</u>, H. Yabu, and <u>M. Shimomura</u>, Novel biomimetic surface based on a self-organized metal–polymer hybrid structure. **Chemistry of Materials** 21, 1799–1801 (2009).

Mimic the structure and functions of natural systems: AIMR researchers succeeded in creating a new biomimetic surface composed of self-organized metal-polymer structures, which can both repel and absorb water droplets like rose petals. They casted a polystyrene-based chloroform solution on a glass substrate, allowed water condensation on the surface in a high-humidity atmosphere, formed a honeycomb membrane with regularly arranged microvoids by vaporizing the chloroform and water droplets, and deposited nickel inside of empty voids on the honeycomb membrane through nonelectrolytic plating. Finally, they peeled off the top layer of the plated honeycomb membrane, which formed a hybrid structure in which micrometer-sized metal domes are distributed on the surface where polymer spikes are arranged. Hydrophilic and hydrophobic domains coexist in this structure. The water droplets placed on its surface are repelled and also absorbed.

*Research results 19 Bio-imaging and bio-sensing devices

*38. <u>Y. Takahashi</u>, A. I. Shevchuk, P. Novak, B. Babakinejad, J. Macpherson, P. R. Unwin, <u>H. Shiku</u>, J. Gorelik, D. Klenerman, Y. E. Korchev and <u>T. Matsue</u>, Topographical and electrochemical nanoscale imaging of living cells using voltage-switching mode scanning electrochemical microscopy. **Proceedings of the**

National Academy of Sciences USA 109, 11540-11545 (2012).

Chemical mapping of living cells: Electroactive and short-lived species that are released and consumed by cells, including neurotransmitters and reactive oxygen-based molecules, are central to cell metabolism; but their detection at cell surfaces and interfaces remains challenging. AIMR researchers have recently developed a high-resolution, non-invasive imaging method called voltage-switching mode—scanning electrochemical microscopy (VSM—SECM), and have succeeded in acquiring high-resolution topographical and electrochemical images of living cells simultaneously. In order to prevent damage to the living cells, they used a faradaic current generated by the reacting electroactive species to control the motion of the electrode, and continuously prevent it from touching the substrate surface. Moreover, they fabricated nanometer-sized glass-insulated carbon electrodes that allow for high-resolution imaging. The next challenge is to monitor the release-related changes in neuron topography.

*39. K. Ino, T. Nishijo, T.Arai, Y. Kanno, <u>Y. Takahashi</u>, <u>H. Shiku</u>, and <u>T Matsue</u>, Local redox-cycling-based electrochemical chip device with deep microwells for evaluation of embryoid bodies. **Angewandte Chemie International Edition** 51, 6648–6652 (2012).

An integrated electrochemical device to monitor stem cells: Embryonic stem cells (ES cells) are useful cells that can differentiate into various cells. AIMR researchers recently have built an integrated electrochemical device that monitors the activity and differentiation of stem cells in an embryoid body. Detection is achieved using an array of 256 (16×16) electrochemical sensors with only 32 (16+16) bonding pads for external connection placed at the base of deep microwells, enabling spatially-resolved measurements. This electrochemical sensor density is the highest in the field of electrochemical lab-on-a-chip devices. The researchers quantified cellular activity from embryoid bodies on the array by collecting local current signals based on 'redox cycling.' They succeeded in getting the signal of the differentiation of the stem cells, and the device will therefore be useful to screen embryoid bodies' differentiation levels.

*Research results 20 Micro Electro Mechanical System (MEMS)

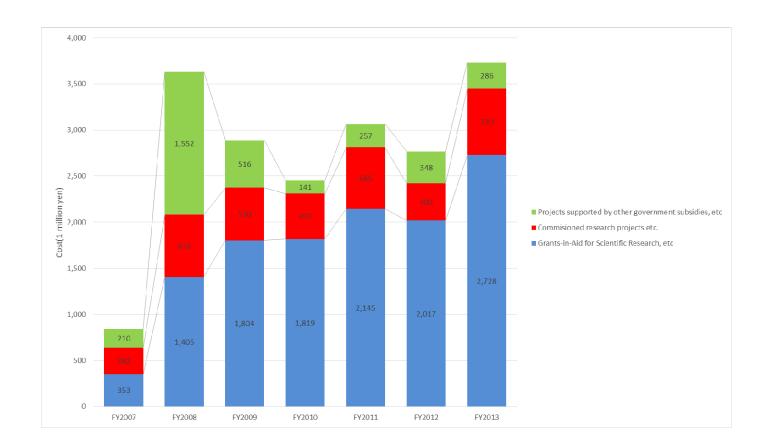
*40. <u>J.-W. Lee, Y.-C. Lin, N. Kaushik, P. Sharma, A. Makino, A. Inoue, M. Esashi</u> and <u>T. Gessner, Micromirror</u> with large-tilting angle using Fe-based metallic glass. **Optics Letters**, 36, 3464-3466 (2011). (This paper overlaps with the interdisciplinary research result shown in Appendix 3.)

BMG suitable for MEMS: Silicon has been traditionally the material of choice in micromechanical innovations. The brittleness of silicon, however, limits the possible range of its applications. The AIMR fusion research team for micro electro mechanical systems (MEMS) and bulk metallic glasses (BMG) used metallic glasses as a tougher and viscous alternative to silicon in the development of enhanced micro-mirrors. They constructed a mirror structure by placing a round mirror plate between two torsion bars that formed the axis for the mirror's movements. The two torsion bars and surface of the round plate were made from BMG. Thanks to the excellent mechanical properties of BMG, the tilt angle of the mirror reached up to 270 degrees in static mode, while up to 70 degrees could be achieved even in dynamic mode with rotational oscillation of more than 300 times per second. Such unique usage was never found in metallic glasses prior to the fusion research in AIMR.

2. Annual transition in non-WPI project funding (grants)

*Make a graph of the annual transition in non-WPI project funding (grants).

^{*}Describe external funding warranting special mention.



[External funding warranting special mention]

- Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST) -

Chief Researcher : Prof. Masayoshi Esashi

Total amount(JPY) (FY2009-FY2013) : 1,557 million yen

• Chief Researcher: Prof. Hideo Ohno

Total amount(JPY) (FY2009-FY2013): 428 million yen

- Creation of Innovation Centers for Advanced Interdisciplinary Research Areas -

• Chief Researcher : Prof. Masayoshi Esashi

Total amount(JPY) (FY2007-FY2013): 2,959 million yen

- Exploratory Research for Advanced Technology-

• Chief Researcher: Prof. Hiroyuki Isobe

Total amount(JPY) (FY2013): 750 million yen

Advanced Environmental Materials Area, Green Network of Excellence (GRENE)
 program sponsored by the Ministry of Education, Culture, Sports, Science and Technology -

• Chief Researcher: Prof. Kazue Kurihara

Total amount(JPY) (FY2011-FY2013): 522 million yen

- Core Research for Evolutionary Science and Technology (CREST) -

• Chief Researcher: Prof. Kazue Kurihara

Total amount(JPY) (FY2009-FY2013): 293 million yen

• Chief Researcher : Prof. Masatsugu Shimomura

Total amount(JPY) (FY2009-FY2013): 172 million yen

• Chief Researcher : Prof. Mingwei Chen

Total amount(JPY) (FY2011-FY2013): 197 million yen

• Chief Researcher: Prof. Motoko Kotani

Total amount(JPY) (FY2011-FY2013): 120 million yen

• Chief Researcher : Prof. Eiji Saitoh

Total amount(JPY) (FY2012-FY2013): 42 million yen

- Gran-in-Aid for Scientific Research Scientific Research (S) -

• Chief Researcher: Prof. Masayoshi Esashi

Total amount(JPY) (FY2007-FY2011): 110 million yen

• Chief Researcher : Prof. Tadafumi Adschiri

Total amount(JPY) (FY2009-FY2011): 131 million yen

• Chief Researcher: Prof. Masahiko Yamaguchi

Total amount(JPY) (FY2009-FY2011): 127 million yen

• Chief Researcher: Prof. Takashi Takahashi

Total amount(JPY) (FY2011-FY2013): 180 million yen

• Chief Researcher: Prof. Shinichi Orimo

Total amount(JPY) (FY2013): 39 million yen

- NEDO Ultra Hybrid material technology and development project (Technology and development of conflicting functional materials based on the nano level structure control) -

• Chief Researcher: Prof. Tadafumi Adschiri

Total amount(JPY) (FY2010-FY2011): 273 million yen

3. Major Awards, Invited Lectures, Plenary Addresses (etc.) (within 2 pages)

3-1. Major Awards

- * List main internationally-acclaimed awards received announced in order from the most recent.
- * For each, write the recipient's name, name of award, and year issued. In case of multiple recipients, underline those affiliated with the center.
- Takashi Takahashi, The 11th Honda Frontier Award, February 2014 (award ceremony: May 2014).
- 2. Kosmas Prassides, Royal Society Wolfson Research Merit Award, February 2014.
- 3. **Ali Khademhosseini**, Elected AAAS(American Association for the Advancement of Science) Fellow, 2013.
- 4. **Alexander Shluger**, 2013 Daiwa Adrian Prizes, 2013.
- 5. **Taro Hitosugi**, Gottfried Wagener Prize 2013, 3rd prize, 2013.
- 6. **Kazue Kurihara**, Selected as the "IUPAC 2013 Distinguished Women in Chemistry or Chemical Engineering", 2013.
- 7. **Hideo Ohno**, Fellow of American Physical Society, 2012.
- 8. Ali Khademhosseini, The 2012 Young Investigator Award, Biochemical Engineering Journal, 2012.
- 9. Hideo Ohno, IEEE David Sarnoff Award, 2012.
- 10. Yuichi Ikuhara, Fellow, The American Ceramic Society, 2011.
- 11. Ali Khademhosseini, Presidential Early Career Award for Scientists and Engineers (PECASE), 2011.
- 12. **Ali Khademhosseini**, Early Career Award in Nanotechnology, The IEEE Nanotechnology Council (NTC), 2011.
- 13. **Alain Reza Yavari**, Award for Scientific Excellence, French National Center for Scientific Research (CNRS), 2011.
- 14. **Kingo Itaya**, The Prix Jacques Tacussel Award of the International Society of Electrochemistry, 2011.
- 15. **Mingwei Chen**, The 2011 Distinguished Award, The 8th International Workshop on Intermetallic and Advanced Materials, China, 2011.
- 16. Yuichi Ikuhara, Humboldt Research Award, 2011.
- 17. Kazue Kurihara, A. E. Alexander Lecture Award 2011, The Royal Australian Chemical Institute, 2011.
- 18. Yoshinori Yamamoto, Centenary Prize 2009, Royal Society of Chemistry, UK, 2009.
- 19. **Toshio Nishi**, International Rubber Conference Organization (IRCO) Medal, 2009.
- 20. Akihisa Inoue, James C. McGroddy Prize for New Materials, American Physical Society, 2009.
- 21. **Terunobu Miyazaki**, Oliver E. Buckley Condensed Matter Prize, American Physical Society, 2009.
- 22. Terunobu Miyazaki, Asahi Prize, 2008.
- 23. Yoshinori Yamamoto, Arthur C. Cope Scholar Award, American Chemical Society, 2007.

3-2. Invited Lectures, Plenary Addresses (etc.) at International Conferences and International Research Meetings

- * List up to 20 main presentations in order from most recent.
- * For each, write the lecturer/presenter's name, presentation title, conference name and date(s)
- Yasumasa Nishiura, "Topological approach in materials science", 2014 NIMS Hot Topics Workshop "British Council Researchers Links Workshop on Soft Matter: Analysis, Applications and Challenges," National Institute for Mathematical Sciences, Daejon, Korea, March 21, 2014 (Plenary Talk)
- 2. **Shin-ichi Orimo**, "Advanced hydride researches for hydrogen and electrochemical energy storages," IUPAC 9th International Conference on Novel Materials and Synthesis, Shanghai, China, October 17-22, 2013 (**Keynote Lecture**)
- Eiji Saitoh, "From spin pumping to spin Seebeck effect," SpinCat workshop 2013, Mainz, Germany, October 9, 2013 (Plenary Address)

- 4. **Motoko Kotani**, "Discrete Geometric Analysis applied to structural understanding of Materials," US-Japan Crossing Boundaries with Informatics from Basic Science to Social Infrastructure, Washington, D.C., U.S.A., July 7-8, 2013 **(Keynote Talk)**
- 5. **Katsumi Tanigaki**, "Fundamental aspects and applications of devices based on carbon materials," Institute on Basic Science Symposium on Nano Materials, Institute of Basic Science, Seoul, Korea June 30 July 4, 2013 (**Plenary Lecture**)
- 6. **Eiji Saitoh**, "Dynamical generation of spin currents," Joint European Magnetic Symposia 2012 (JEMS2012), Palma, Italia, September 12, 2012 (**Semi Plenary**)
- 7. **Hideo Ohno**, "Bridging Semiconductor and Magnetism," 31st International Conference on the Physics of Semiconductors (ICPS 2012), Zurich, Switzerland, July 29 August 3, 2012 (**Plenary Address**)
- 8. **Tadafumi Adschiri**, "Supercritical Route for Super Hybrid Materials," ISSF 10th International Symposium on Supercritical Fluids, San Francisco, CA, USA, May 13–16, 2012 **(Keynote Lecture)**
- Thomas P. Russell, "Big Things Come in Small Packages," Fred Kavli Distinguished Lectureship in Nanoscience at the 2012 MRS Spring Meeting, San Francisco, April 9, 2012
- 10. **Masatsugu Shimomura**, "New trends in next generation biomimetics: Innovative paradigm shift based on biodiversity," 2012 International Symposium on Nature-Inspired Technology, Kangwon, Korea, January 9-11, 2012 **(Keynote Presentation)**
- 11. **Tomokazu Matsue**, "Highly-Sensitive Electrochemical Imaging for Biosensing," US-Japan Workshop on Bio-Inspired Engineering of Next-Generation Sensors and Actuators, San Francisco, USA, November 12-13, 2011 (Keynote Presentation)
- 12. **Yuichi Ikuhara**, "HAADF and ABF STEM Characterization of Ceramic Interfaces," TEM Workshop Electron Microscopy, Exploring Materials on the Atomic Scale, TU Darmstadt, October 10, 2011 **(Plenary Lecture)**
- 13. <u>Dmitry V. Louzguine-Luzgin</u>, <u>K. Georgarakis</u>, J. Antonowicz, G. Vaughan, <u>A.R. Yavari</u>, <u>T. Egami</u>, <u>A. Inoue</u>, "Changes in Atomic Structure of Supercooled Pd-Ni-Cu-P Glassforming Liquid during in-situ Vitrification on Cooling Established by Synchrotronradiation X-ray Diffraction," Euromat 2011, Montpellier, France, September 12-15, 2011 (Keynote Presentation)
- 14. **Tadafumi Adschiri**, "Supercritical Route for Super Hybrid Nanomaterials," International Conference on Materials for Advanced Technologies (ICMAT 2011), Singapore, June 27 July1, 2011 **(Keynote Presentation)**
- 15. Kazue Kurihara, "Surface Forces Measurement for Nano-Materials Science" as the A. E. Alexander Lecture, Australian Colloid and Interface Symposium (ACIS) 2011, Hobart, Australia, January 30 -February 3, 2011
- 16. **Katsumi Tanigaki**, "What we have learned from Fullerenes: From the viewpoint of physical parameters," Fullerene Silver Anniversary Symposium, Crete, Greece, October 4-10, 2010 **(Keynote Lecture)**
- 17. **Masaru Tsukada**, "Theoretical Approaches for the Analyses of Scanning Probe Microscopy," **Tutorial talk** at 7th International Symposium on Atomic Level Characterizations for New Materials and Devices '09 (ALC '09), Maui, Hawaii, USA, December 6-11, 2009
- 18. **Yoshinori Yamamoto**, "From sigma to pi Electrophilic Lewis Acids. Application to Selective Organic Transformations," **RSC Centenary Prizes Lectures** at Univ. York (October 12), at Univ. Belfast (October 14), and at Durham Univ. UK, October 16, 2009.
- 19. **Masayoshi Esashi**, "MEMS for Test and Instrumentation," 9th International Conference on Electronic Measurement and Instruments (ICEMI 2009), Beijing, August16, 2009 (**Plenary Talk**)
- 20. **Mingwei Chen**, "Structure and Properties of Nanoporous metals," International Conference on Frontiers in Materials Science & Technology (FMST2008), Brisbane, Australia, March 26-28, 2008 (**Keynote Lecture**)

4. List of Achievements of Center's outreach activities

* Using the table below, show the achievements of the Center's outreach activities from FY2011 through FY2013 (number of activities, times held).

Activities	FY2011 (number of activities, times held)	FY2012 (number of activities, times held)	FY2013 (number of activities, times held)
PR brochure, pamphlet	13	5	7
Lectures, seminars for general public	22	4	7
Teaching, experiments, training for elementary and secondary school students	5	7	17
Science cafe	0	3	3
Open houses	5	2	2
Participating, exhibiting in events	13	6	13
Press releases	28	26	26

5. List of Media Coverage of Projects Carried Out between FY2011-2013 (within 2 pages)

1) Japan

No.	Date	Type media (e.g., newspaper, magazine, television)	Description
1	2014/3/9 2014/2/6 2014/2/1	Nikkei Nikkei Sangyo Shimbun Kahoku Shimpo	Successful imaging of the atomic structure of shark teeth (Ikuhara)
2	2013/12/25	Asahi Shimbun	Relay Opinion "Spirits of Rikejo to the next generation" (Interview with Director Kotani)
3	2013/12/14	[TV] NHK (News)	Science Talk Live 2013 by WPI (WPI Joint Symposium)
4	2013/11/27 2013/11/15	Nikkei Sangyo Shimbun Nikkan Kogyo Shimbun	Theoretically clarified the factors involved in preventing charge loss in organic thin film solar cells (Tamura)
5	2013/11/25	[Magazine] Nikkei Science	Front Runner (Interview with Director Kotani)
6	2013/10/31	Yomiuri Shimbun, Nikkan Kogyo Shimbun	12 centers were selected for the COI Stream (Matsue)
7	2013/10/29 2013/9/17	[TV] NHK Educational (Suiensaa)	Challenge from Tohoku University (Director Kotani as chairman)
8	2013/9/22 2013/9/12	[TV] BS11 (Weekly News Onze) Yomiuri Shimbun, Mainichi Shimbun, Nikkei Sangyo Shimbun	Akari Takayama was awarded by the L'Oréal-UNESCO Japan Fellowship
9	2013/8/31	[TV] TBS (Mirai no Kigen)	Nanotechnology can change medical care (Fujie)
10	2013/8/11 2013/7/12	Nikkei Kahoku Shimpo, Nikkei Sangyo Shimbun	Perfect distortion: geometric frustration of icosahedron for glass formation (Chen, Kotani)
11	2013/7/1	[TV] NHK (Today's Close-up)	Learning from nature for innovation (Shimomura)
12	2013/4/16	Asahi Shimbun, Mainichi Shimbun, Shizuoka Shimbun, Nikkei, Jiji, Nikkan Kogyo Shimbun, Nikkei Sangyo Shimbun, [TV] NHK, NTV (News)	Successful high-resolution scanning electron microscopy of living organism (Shimomura)
13	2013/3/12	Nikkan Kogyo Shimbun, Nikkei Sangyo Shimbun, Dempa Shimbun	A new guideline for developing novel functional hydrides (Orimo)
14	2013/1/17	Nikkei	Special Issue for Advanced Institute for Materials Research
15	2012/11/6	Nikkei, Nikkei Sangyo Shimbun, Nikkan Kogyo Shimbun	Success in fabricating graphene intercalation compound (Takahashi, Hitosugi)

^{*} Select main items of press releases, media coverage, and reports (especially overseas)

			,
16	2012/9/24 2012/9/21	Nikkei Sangyo Shimbun Nikkan Kogyo Shimbun	World record achieved in superconducting transition temperature of transparent superconductor (Hitosugi)
17	2012/6/25 2012/6/18	[TV] NHK Educational (Test no Hanamichi)	Campus Tour, Tohoku University (Takahashi, Hitosugi)
18	2012/6/18	Asahi Shimbun	NEC and Tohoku University develop a new device for generating electricity from easily-accessible heat sources (Saitoh)
19	2012/6/12 2012/6/11	Nikkan Kogyo Shimbun, Kahoku Shimpo Yomiuri Shimbun	Development of low power consumption memory (Ohno)
20	2012/6/4	Nikkan Kogyo Shimbun, Nikkei Sangyo Shimbun, Kahoku Shimpo	Silicon quantum dot solar cell, conversion efficiency of 12.6% (Samukawa)
21	2012/5/24	Yomiuri Shimbun	Development of spintronics (Ohno)
22	2011/12/4 2011/11/17	Yomiuri Shimbun, Chunichi Shimbun, Tokyo Shimbun, Nikkei Sangyo Shimbun, Nikkan Kogyo Shimbun	Discovery of an unexpected superstructure in an oxide (Ikuhara)
23	2011/11/9 2011/11/5	Nikkei, Kahoku Shimpo Nikkei	Tohoku University makes an agreement with a German research institute and promotes exchange activities in advanced technology. (Esashi)

2) Overseas

No.	Date	Type media (e.g., newspaper, magazine, television)	Description
1	2014/1/29 2014/1/27	Chemistry Views Chemical & Engineering News	Successful imaging of the atomic structure of shark teeth (Ikuhara)
2	2013/11/12 2013/10/25 2013/10/24	Science News Chemistry World materials360 online	Water squishes into stable shapes, no container required (Russell)
3	2013/7/15	Physics World Microscopy analysis	Perfect distortion: geometric frustration of icosahedron for glass formation (Chen, Kotani)
4	2013/4/29	Phys.org Science Daily	Bioengineers create rubber-like material bearing micropatterns for stronger, more elastic hearts (Khademhosseini)
5	2013/4/22	Physics World	Successful heat energy conveyance using magnetic waves (Saitoh)
6	2013/2/25	Fox News	Rise of the machines? New steps toward bionic humans (Khademhosseini)
7	2012/8/30	Physics World	Special Report Japan
8	2012/2/14	[TV] CBS News	Boston Researchers Work To Grow Human Organs (Khademhosseini)
9	2011/6/28	EL COMERCIO	We must reduce the cost of nanomaterials for society's use (Yavari)

List of papers of representative of interdisciplinary research activities

1. <u>A. Hirata, L. J. Kang, T. Fujita, B. Klumov, K. Matsue, M. Kotani, A. R. Yavari, M. W. Chen:</u> Geometric frustration of icosahedron in metallic glasses. **Science** 341, 376-379 (2013). (This paper overlaps with the paper shown in Appendix 2.)

The fusion research team of mathematicians and experimentalists at AIMR successfully characterized the atomic structure in metallic glass and revealed atomic-scale competition in energy and geometry for glass formation. The experimenters developed an angstrom beam electron diffraction method, analyzing the local atomic structure. Mathematicians applied "computational homology" to analyze the observed structure. This collaboration unveiled the long-standing mystery of atomic configurations: that geometric distortions of icosahedral clusters in metallic glass can be scaled up to long-range disorder with topological connectivity. The co-existence of icosahedral and FCC-crystal-like symmetries in the distorted icosahedral clusters leads to the perfect distortion for making a disordered, densely-packed structure. The underlying discrepancy that remained unknown for half a century has been resolved.

2. <u>D. M. Packwood</u>, <u>S. Shiraki</u>, and <u>T. Hitosugi</u>: Effects of Atomic Collisions on the Stoichiometry of Thin Films Prepared by Pulsed Laser Deposition. **Physical Review Letters** 111, 036101 (2013)

In this study, a fusion research team made up of a theoretical chemist belonging to Interface Unit and experimental materials scientists at AIMR succeeded in developing a promising analytic model to quantitatively describe the cation nonstoichiometry in the pulsed laser deposition process of oxide films. This is the first analytic model of collision-induced plume expansion that can predict the partial oxygen pressure dependence of the Li content of a thin film. This model gives us very important implications for collision effects that affect the growth of thin films containing both light and heavy elements. For the demonstration, deposited thin films via the ablation of Li_{1.3}Mn₂O₂ targets under various oxygen pressures showed good agreement with the compositions predicted by the model. This gives us a guiding principle to accurately control oxide stoichiometry, which is extremely important for high quality films.

3. T. Matsuno, H. Naito, S. Hitosugi, <u>S. Sato, M. Kotani, H. Isobe,</u> Geometric measures of finite carbon nanotube molecules: a proposal for length index and filling indexes. **Pure and Applied Chemistry** 86, 489–495 (January 2014).

A research group from AIMR has proposed new geometric measures for finite carbon nanotube (CNT) molecules. Although geometric measures for CNT, such as a chiral index using the coordinates (n,m), were first proposed in 1992 and widely accepted by various fields, a measure for finite CNT molecules was unavailable because of the absence of such molecular entities. In recent years, with the appearance of finite carbon nanotubes with discrete sizes, the need for an index to measure length and bond-filling and atom-filling rates has increased. AIMR dealt with this problem as fusion research with mathematicians (geometricians) and succeeded in obtaining a new index. The newly proposed geometric index is hoped to be a basis for the development of science and technology related to finite CNT molecules.

^{*} List up to 20 papers that underscoring each interdisciplinary research activity and give brief accounts (within 10 lines).

^{*} For each, write the author name(s); year of publication; journal name, volume, page(s), and article title. Any listing order may be used as long as format is the same. If a paper has many authors, underline those affiliated with the Center.

^{*} If a paper has many authors (say, more than 10), all of their names do not need to be listed.

4. <u>D. M. Packwood</u>, K. T. Reaves, <u>F. L. Federici</u>, H. G. Katzgraber, and <u>W. Teizer</u>, Two-dimensional molecular magnets with weak topological invariant magnetic moments: Mathematical prediction of targets for chemical synthesis. **Proceedings of the Royal Society A** 469, 20130373 (2013).

Molecular magnets can be handled like classical particles owing to their relatively large size, but they also exhibit quantum magnetic properties thanks to their unpaired electron spins. This unique behavior makes them attractive as material for high-density information storage and spintronic-based computing. Currently, chemists struggle to attach molecular magnets to device surfaces. However, these particles have a tendency to warp and lose their magnetic properties upon adsorption. To overcome this difficulty, fusion research between experimental materials scientists and a theoretical chemist belonging to the Interface Unit has been carried out, and they developed innovative "mathematical chemistry" techniques that can predict the structure of novel molecular magnets with deformation-resistant magnetic moments.

5. <u>D. V. Louzguine-Luzgin</u>, <u>D. M. Packwood</u>, G. Xie, A. Y. Churyumov, On deformation behavior of a Ni-based bulk metallic glass produced by flux treatment. **Journal of alloys and compounds** 561, 241-246 (2013).

A fusion research team of a theoretical chemist belonging to Interface Unit and experimental materials scientists analyzed the deformation of BMG. They produced $Ni_{50}Pd_{30}P_{20}$ bulk metallic glass by flux treatment and casing, and confirmed the formation of a glassy structure of the alloy by X-ray diffraction and transmission electron microscopy. Its deformation behavior under uniaxial compression at room temperature was studied at the strain rate of $5x\ 10^{-4}\ s^{-1}$, as well as at three different strain rates at quasistatic loading conditions. The serrated flow behavior appeared to be chaotic, and was analyzed with a stochastic model. The model suggests that the underlying serrated slow dynamics initially result from the appearance of new shear bands in the material; but as the experiment proceeds, the nature of these dynamics change, and strain takes place through the enlargement of shear bands already present on the material.

6. <u>R. Iguchi, K. Sato, D. Hirobe, S. Daimon, and E. Saitoh, Effect of spin Hall magnetoresistance on spin pumping measurements in insulating magnet/metal systems. **Applied Physics Express** 7, 013003 (January 2014).</u>

It is known that a DC rectification effect of AC voltage by magnetization dynamics occurs in systems where magnetoresistance exists. A fusion research team between experimental researchers and a theoretical physicist belonging to the Interface Unit investigated the DC rectification effect of magnetization dynamics based on spin Hall magnetoresistance (SMR) in an insulating magnet/metal system on spin pumping measurements. They theoretically found that the rectification effect due to SMR has a different in-plane magnetization angle dependence from that of the inverse spin Hall effect on the spin pumping. The negligible contribution from the rectification effect was experimentally confirmed in a cavity measurement.

7. <u>Y.H. Liu, D. Wang, K. Nakajima, W. Zhang, A. Hirata, T. Nishi, A. Inoue, and M.W. Chen, Characterization of nanoscale mechanical heterogeneity in a metallic glass by dynamic force microscopy. **Physical Review Letters** 106, 125504 (2011).</u>

One emerging result was obtained through the fusion research of BMG Group and Soft Materials (Polymer) Group. It is becoming clear that shear transformation zones (STZs) on a nanometer scale in BMG have great effects on mechanical characteristics of BMG. On the other hand, the Polymer Group from AIMR has succeeded in mapping the energy dissipation derived from the viscosity in nanoscale areas using AFM, and this method was applied to observe heterogeneity in BMG. The analysis revealed that the non-uniform structure of the viscosity measured in BMG had a distinctive scale of 2.5 nm, which matched that of STZs, suggesting the deep relationship between such inhomogeneity and STZs. There is some similarity between STZs in BMGs and "cooperatively rearranging region (CRR)" in polymer glass, and this will lead to the discovery of common principles that bridge different material systems.

- 8. N. Asao, Y. Ishikawa, N. Hatakeyama, Menggenbateer, Y. Yamamoto, M. W. Chen, W. Zhang and A. Inoue, Nanostructured materials as catalysts: Nanoporous-gold-catalyzed oxidation of organosilanes with water. **Angewandte Chemie International Edition** 49, 10093–10095 (2010). (This paper overlaps with the paper shown in Appendix 2.)
 - It is becoming clear that nanoporous metals created through electrochemical treatment (dealloying treatment) function as highly efficient catalysts. The fusion research team of Bulk Metallic Glasses and Soft Materials Group used nanoporous gold that was obtained by selectively dissolving the silver part of a gold-silver alloy, revealing that the oxidation reaction of organic silane compounds was promoted at room temperature, and that the catalyst can be reused multiple times without degrading its catalytic properties. Conventional attempts have created gold nanoparticles supported on a substrate. However, these particles have a short lifespan owing to agglomeration, and the recovery process was cumbersome. There are great expectations for our nanoporous metallic catalyst in future applications.
- 9. <u>T. Fujita, P. Guan, K. McKenna, X. Lang, A. Hirata, L. Zhang, T. Tokunaga, S. Arai, Y. Yamamoto, N. Tanaka, Y. Ishikawa, N. Asao, Y. Yamamoto, J. Erlebacher and M. W. Chen, Atomic origins of the high catalytic activity of nanoporous gold. **Nature Materials** 11, 775–780 (2012).</u>
 - Although the catalytic activity of nanoporous gold towards molecular oxygen is attracting much attention, the underlying mechanism for this catalytic activity remains unclear. The fusion research team consisting of metallurgists and chemists at AIMR recently has captured a new evidence that small defects on gold surfaces are active sites for CO oxidation reactions. Specifically, they observed nanoporous gold *in situ* during a CO oxidation reactions using the spherical-aberration-corrected scanning transmission electron microscopy (Cs-corrected STEM) and by carefully controlling gas pressures. Along bent portions of the nanopores, these steps fell out of alignment and became 'kinks' of under-coordinated gold atoms, which were exceedingly active sites for chemical oxidation. This finding will be able to boost the longevity and activity of gold catalysts.
- M. Yan, <u>T. Jin, Y. Ishikawa</u>, T. Minato, <u>T. Fujita</u>, <u>L.-Y. Chen</u>, M. Bao, <u>N. Asao</u>, <u>M. W. Chen</u> and <u>Y. Yamamoto</u>, Nanoporous gold catalyst for highly selective semihydrogenation of alkynes: remarkable effect of amine additives. **Journal of the American Chemical Society** 134, 17536–17542 (2012).
 - Although nanoporous gold catalysts have gained popularity, due to their long lifespans and their green technology potential, it has been thought that they are inactive in reductive hydrogenation reactions. The fusion research team consisting of metallurgists and chemists showed that this catalyst can be used in the selective hydrogenation of alkynes to alkenes, where carbon–carbon triple bonds are reduced to double bonds. Interestingly, the reaction is both chemoselective and Z-selective. This means that the catalyst can stop the reduction at the double bond state, and the two hydrogen atoms added to the alkyne moiety are always placed on the same side of the bond, forming a highly active isomer known as a Z-alkene. It is expected that nanoporous gold will not only be used in the selective reduction of various functional groups, but will also open opportunities for applications in heterogeneous catalysis for clean chemical synthesis.
- 11. S. Tanaka, T. Kaneko, N. Asao, Y. Yamamoto, M.W. Chen, W. Zhang and A. Inoue, A nanostructured skeleton catalyst: Suzuki-coupling with a reusable and sustainable nanoporous metallic glass Pd-catalyst. **Chemical Communications** 47, 5985–5987 (2011).
 - Palladium is a well-known catalyst for organic synthesis. Unfortunately, palladium catalysts are toxic, expensive, and difficult to separate completely from a final product. The synthetic chemist group (Soft Materials group) of AIMR started to collaborate on palladium catalysts with the Bulk Metallic Glasses (BMG) group, making it possible to create nanoporous palladium with a uniform distribution of pores of about 30 nanometers in diameter by using palladium—nickel—phosphorus

metallic glass and electrochemical fabrication techniques. Consequently, they succeeded in developing a solid palladium-based "metallic glass" that can repeatedly catalyze carbon coupling reactions with negligible leaching of the catalyst into the solvent.

12. K. Kanetani, <u>K. Sugawara</u>, T. Sato, <u>R. Shimizu</u>, <u>K. Iwaya</u>, <u>T. Hitosugi</u> and <u>T. Takahashi</u>, Ca intercalated bilayer graphene as a thinnest limit of superconducting C₆Ca. **Proceedings of the National Academy of Sciences USA** 109, 19610–19613 (2012).

The insertion of substances between its graphene layers to form "graphite intercalation compounds" (GICs) has been investigated as a method for the storage of lithium atoms within batteries. Interestingly, some GICs can also become superconductive. The fusion research team consisting of physicists, chemists, and surface scientists at AIMR recently has constructed a carbon-based superconductor C_6Ca at its two-dimensional limit by trapping calcium atoms between just two layers of graphene. Their "sandwich" material offers the advantages of bulk graphite while being as thin as it can possibly be. Among the known superconducting GICs, C_6Ca is arguably the most interesting, as it develops superconductivity at a higher temperature than any other. This research area should help to gain a fundamental understanding of the physical and chemical process relevant to state-of-the-art batteries, using graphite as an electrode.

13. <u>H. Chang</u>, Z. Sun, <u>M. Saito</u>, Q. Yuan, H. Zhang, J. Li, <u>Z. Wang</u>, <u>T. Fujita</u>, F. Ding, Z. Zheng, F. Yan, <u>H.-K. Wu</u>, <u>M. W. Chen</u>, and <u>Y. Ikuhara</u>, Regulating infrared photoresponses in reduced graphene oxide phototransistors by defect and atomic structure control. **ACS Nano** 7, 6310–6320 (2013).

Graphene is a promising material also for application to photodetectors due to its exceptional electronic properties. However, the electrons and holes rapidly recombine in graphene. As a result, the amount of photocurrent generated from incident radiation (the photoresponse) is very low, and preparing a graphene-based photodetector has remained a challenge. In this study, a fusion research team of the researchers from Device/System, Bulk Metallic Glasses, and Materials Physics groups from AIMR, has demonstrated the possibility of enhancing the infrared photoresponse of graphene oxide, a close relative of graphene, by controlling the structure and number of defects in the material. By thermal annealing, they controlled the surface oxidation state and succeeded in detecting a photocurrent signal and fabricating flexible infrared test detection devices which do not break upon bending.

14. Y. Yamada, <u>K. Ueno</u>, T. Fukumura, H.T. Yuan, H. Shimotani, Y. Iwasa, L. Gu, <u>S. Tsukimoto</u>, <u>Y. Ikuhara</u> and <u>M. Kawasaki</u>, Electrically induced ferromagnetism at room temperature in cobalt-doped titanium dioxide. **Science** 332, 1065-1067 (2011).

Integrating ideas and techniques among materials scientists specializing in semiconductors, device physicists skilled in electric double layer transistors, chemists operating liquid electrolytes, and physicists specializing in microscopy have led to new possibilities for utilizing "spin." The ability to switch the magnetic properties or electron "spin" of a semiconductor, in a similar vein to charge in conventional devices, opens up new possibilities for fast, low-power data storage and "spintronics" applications. The researchers have developed a magnetic semiconductor system with controllable ferromagnetism at room temperature. They used TiO₂ containing a small amount of the magnetic element cobalt, and injected a high concentration of charge by using a liquid electrolyte. The development of a magnetic semiconductor providing switchable magnetic properties at room temperature offers intriguing possibilities for high-performance devices.

15. <u>K.S. Nakayama</u>, <u>Y. Yokoyama</u>, T. Ono, <u>M.W. Chen</u>, K. Akiyama, <u>T. Sakurai</u> and A. Inoue, Controlled formation and mechanical characterization of metallic glassy nanowires. **Advanced Materials** 22, 872–875 (2010). (This paper overlaps with the paper shown in Appendix 2.)

This paper showed the capability of metallic glasses for creating nanowires and their useful application. As opposed to crystalline nanomaterials, metallic glasses have no defects or grain

boundaries. When it is heated above the glass transition temperature, its viscosity suddenly drops, enabling super-plastic deformation which enables the creation of long nanowires by extension. The lack of grain boundaries also helps the long extension of the wire. AIMR researchers succeeded in creating metallic glass nanowires of less than 40 nm in diameter by exploiting this property. In collaboration with the micro electro mechanical systems (MEMS) laboratory, they have succeeded in derivation of Young's modulus with the resonant measurement of the metallic glass nanowires, thus opening up possibilities for application to nanoresonators.

16. <u>J.-W. Lee, Y.-C. Lin, N. Kaushik, P. Sharma, A. Makino, A. Inoue, M. Esashi</u> and <u>T. Gessner, Micromirror with large-tilting angle using Fe-based metallic glass. **Optics Letters**, 36, 3464-3466 (2011). (This paper overlaps with the paper shown in Appendix 2.)</u>

Silicon has been traditionally the material of choice in micromechanical innovations. The brittleness of silicon, however, limits the possible range of its applications. The AIMR fusion research team for MEMS and bulk metallic glasses (BMG) used metallic glasses as a tougher and viscous alternative to silicon in the development of enhanced micro-mirrors. They constructed a mirror structure by placing a round mirror plate between two torsion bars that formed the axis for the mirror's movements. The two torsion bars and surface of the round plate were made from BMG. Thanks to the excellent mechanical properties of BMG, the tilt angle of the mirror reached up to 270 degrees in static mode, while up to 70 degrees could be achieved even in dynamic mode with rotational oscillation of more than 300 times per second. Such unique usage was never found in metallic glasses prior to the fusion research in AIMR.

17. <u>S. Ahadian</u>, <u>J. Ramon-Azcon</u>, M. Estili, X. B. Liang, <u>S. Ostrovidov</u>, <u>H. Shiku</u>, <u>M. Ramalingam</u>, <u>K. Nakajima</u>, Y. Sakka, H. Bae, <u>T. Matsue</u>, <u>A. Khademhosseini</u>, Hybrid hydrogels containing vertically aligned carbon nanotubes with anisotropic electrical conductivity for muscle myofiber fabrication. **Scientific Reports** 4, 4271 (March 2014).

Biological scaffolds with tunable electrical and mechanical properties are required in many fields, such as regenerative medicine, biorobotics, and biosensing. In this study, a fusion research team of biomaterials, polymers, and biodevices used dielectrophoresis (DEP) to vertically align carbon nanotubes (CNTs) within methacrylated gelatin (GelMA) hydrogels in a robust, simple, and rapid manner. GelMA-aligned CNT hydrogels showed anisotropic electrical conductivity and superior mechanical properties compared with pristine GelMA hydrogels and GelMA hydrogels containing randomly distributed CNTs. Skeletal muscle cells grown on vertically aligned CNTs in GelMA hydrogels yielded a higher number of functional myofibers than cells that were cultured on hydrogels with randomly distributed CNTs and horizontally aligned CNTs, as confirmed by the expression of myogenic genes and proteins.

18. <u>L. Zhang</u>, <u>H. Chang</u>, <u>A. Hirata</u>, <u>H. Wu</u>, <u>Q.-K. Xue</u>, and <u>M. W. Chen</u>, Nanoporous gold based optical sensor for sub-ppt detection of mercury ions. **ACS Nano** 7, 4595–4600 (2013).

As mercury is harmful to humans, its concentration in tap water is monitored closely. However, detecting sub-part-per-trillion levels of mercury ions with high sensitivity is difficult, and still challenging. A fusion research team of Materials Physics group (AIMR and Tsinghua Univ.), Bulk Metallic Glasses group and Device/System group designed a nanoporous gold-based optical sensor about 1,000 times more sensitive than conventional optical methods by utilizing the surface-enhanced resonance Raman scattering (SERRS) technique. Since the intensity of SERRS depends on the surface area of the specimen, the team used nanoporous gold as a substrate. The fluorochrome reporter molecule cyanine 5 (Cy5) is detected, rather than the mercury ion itself, and the existence of a trace amount of mercury appeared as a reduction in the SERRS signal intensity. This result reveals a new mechanism for mercury detection.

19. <u>K. Oniwa, T. Kanagasekaran, T. Jin, Md. Akhtaruzzaman, Y. Yamamoto, H. Tamura, I. Hamada, H. Shimotani, N. Asao, S. Ikeda, and K. Tanigaki, Single crystal biphenyl end-capped</u>

furan-incorporated oligomers: influence of unusual packing structure on carrier mobility and luminescence. **Journal of Materials Chemistry C** 1, 4163–4170 (2013).

Organic light-emitting field-effect transistors (OLETs) are innovative devices combining light emissions with electronic switching, based on the ambipolar characteristics of organic semiconductors. Although OLETs are expected to be applied to all-organic lasers, it has so far been inhibited by a problem: the π - π stacking that boosts the mobility of charge carriers generally stifles light emissions in a trade-off manner. The interdisciplinary fusion research team of experimental physicists, synthetic chemists, and theoretical chemists/physicists synthesized new oligomer BPFTs by substituting one thiophene ring in BP2T with a furan ring. They found that BPFT shows about 30% higher luminescence efficiency than that of BP2T, while BPFT preserves the same level of carrier mobility. Theoretical discussion about the higher luminescence efficiency observed in BPFT is described in detail in the following paper (no. 20).

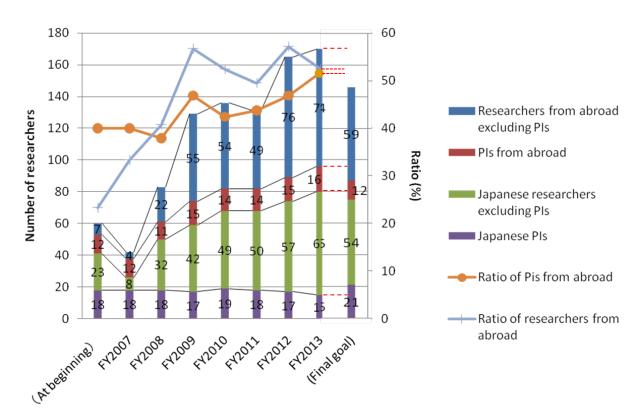
H. Tamura, I. Hamada, H. Shang, K. Oniwa, Md. Akhtaruzzaman, T. Jin, N. Asao, Y. Yamamoto, T. Kanagasekaran, H. Shimotani, S. Ikeda, and K. Tanigaki. Theoretical analysis on the optoelectronic properties of single crystals of thiophene-furan-phenylene co-oligomers: efficient photoluminescence due to molecular bending. The Journal of Physical Chemistry C 117, 8072–8078 (2013).

This paper dealt with the experimental result of paper no. 19, based on theoretical calculations. Using the molecular structure and crystal structure experimentally determined (by single crystal X-ray diffraction analysis), the electronic structure was calculated by density functional theory (DFT), and the mechanism of the higher luminescence efficiency in BPFT than BP2T was discussed. The unit cell of a BPFT crystal consists of two molecules, where one molecule bends in the unit cell. This bend of one molecule breaks the equilibrium inherent to aromatic solids, causing asymmetric electronic dipoles to form during the transition to a photo-excited state. These dipoles generate luminescent emissions that are forbidden in totally symmetric complexes like BP2T. The cooperation between theoreticians and experimentalists led to the new idea to simultaneously improve the luminescence efficiency and carrier mobility of organic crystals.

World Premier International Research Center Initiative (WPI)

1. Number of overseas researchers and annual transition

*Make a graph of the transition in the number of overseas researchers since the application.



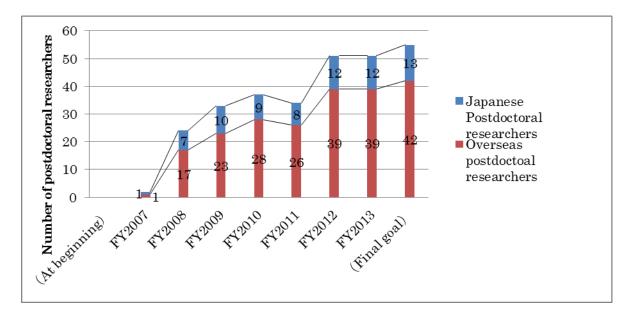
2. Postdoctoral positions through open international solicitations

* In the column of number of applications and number of selection, put the number and percentage of overseas researchers in the < > brackets.

FY	number of applications	number of selection	
FY2007	0 < , %>	0 < , %>	
FY2008	6 < 5, 83%>	3 < 3, 100%>	
FY2009	7 < 5, 71%>	5 < 5, 100%>	
FY2010	68 < 58, 85%>	11 < 10, 90%>	
FY2011	38 < 35, 92%>	6 < 6, 100%>	
FY2012	250 < 163, 65%>	10 < 5, 50%>	
FY2013	97 < 83, 86%>	7 < 5, 71%>	

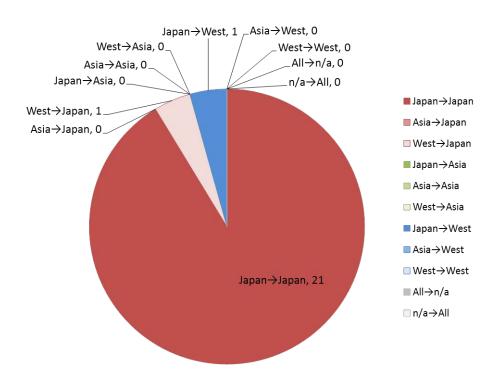
3. Number of overseas postdoctoral researchers and annual transition

*Make a graph of the transition in the number of overseas postdoctoral researchers since the application.

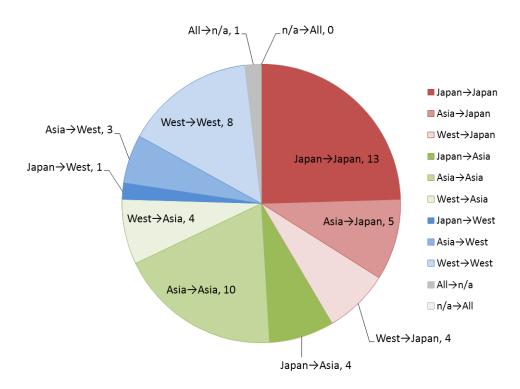


- 4. Status of postdoc employment at institutions of postdoctoral researchers
- OO \rightarrow Δ indicates that a posdoc has come to the WPI Center from an institute in OO and moved to one in Δ Δ .
- n/a indicates unknown or resignation for personal reason.

Japanese Postdocs



Overseas Postdocs



5. List of the cooperative research agreements outside Japan

1. **Counterpart of an Agreement:** Faculty of Mathematical and Physical Sciences (MAPS), University College London

Name of an Agreement: MEMORANDUM OF COLLABORATION BETWEEN faculty of Mathematical and Physical Sciences (MAPS) UNIVERSITY COLLEGE LONDON, UK AND The WPI-Advanced Institute for Materials Research (WPI-AIMR) Tohoku University, Japan

Dates of an Agreement: January 6, 2009

Summary of an Agreement:

- To establish collaborative research in areas relating to Materials research
- To work together for the of organisation of workshops
- To facilitate exchange of staff and students
- To facilitate the exchange of research materials between the institutions
- To identify ways of making these exchanges viable involving specialized researchers
- Counterpart of an Agreement: The Department of Materials Science and Metallurgy (MSM), University of Cambridge

Name of an Agreement: AGREEMENT ON ACADEMIC EXCHANGE BETWEEN THE WORLD PREIER INTERNATIONAL RESEARCH CENTER ADVANCED INSTITUTE FOR MATERIALS RESEARCH (WPI-AIMR) TOHOKU UNIVERSITY, JAPAN AND THE DEPARTMENT OF MATERIALS SCIENCE AND METALLURGY (MSM) UNIVERSITY OF CAMBRIDGE, UNITED KINGDOM

Dates of an Agreement: January 26, 2010

Summary of an Agreement:

- Promotion of joint research and educational activities
- Invitation to short-term visits of researchers for academic activities
- Exchange of information and pertinent publication in fields of interest to both universities
- Exchange of faculty members, researchers and students for study and research
- 3. Counterpart of an Agreement: World Class University(WCU): Division of Advanced Materials Science (AMS), Pohang University of Science & Technology (POSTECH)

 Name of an Agreement: AGREEMENT ON ACADEMIC EXCHANGE BETWEEN WORLD PREMIER INTERNATIONAL RESEARCH CENTER (WPI): ADVANCED INSTITUTE FOR MATERIALS RESEARCH (WPI-AIMR), TOHOKU UNIVERSITY, JAPAN AND WORLD CLASS UNIVERSITY (WCU): DIVISION OF ADVANCED MATERIALS RESEARCH (WCU-AMS), POHANG UNIVERSITY OF SCIENCE & TECHNOLOGY (POSTECH), KOREA

Dates of an Agreement: March 27, 2010

Summary of an Agreement:

- Promotion of joint research and educational activities
- Invitation to short-term visits of researchers for academic activities
- Exchange of information and pertinent publication in fields of interest to both universities
- Exchange of faculty members, researchers and students for study and research
- 4. **Counterpart of an Agreement:** School of Science, The Hong Kong University of Science and Technology

Name of an Agreement: AGREEMENT ON ACADEMIC EXCHANGE BETWEEN WORLD PREMIER INTERNATIONAL RESEARCH CENTER – ADVANCED INSTITUTE FOR MATERIALS RESEARCH (WPI-AIMR), TOHOKU UNIVERSITY, JAPAN AND SCHOOL OF SCIENCE, HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY, CHINA

Dates of an Agreement: April 1, 2010

Summary of an Agreement:

- Promotion of joint research and educational activities
- Invitation to short-term visits of researchers for academic activities

- Exchange of information and pertinent publication in fields of interest to both universities
- Exchange of faculty members, researchers and students for study and research
- 5. **Counterpart of an Agreement:** Institute of Chemistry, Chinese Academy of Sciences **Name of an Agreement:** AGREEMENT ON ACADEMIC EXCHANGE BETWEEN WORLD PREIER INTERNATIONAL RESEARCH CENTER ADVANCED INSTITUTE FOR MATERIALS RESEARCH (WPI-AIMR) TOHOKU UNIVERSITY, JAPAN AND INSTITUTE OF CHEMISTRY, CHINESE ACADEMY OF SCIENCES, CHINA

Dates of an Agreement: April 10, 2010

Summary of an Agreement:

- Promotion of joint research and educational activities
- Invitation to short-term visits of researchers for academic activities
- Exchange of information and pertinent publication in fields of interest to both universities
- Exchange of faculty members, researchers and students for study and research
- 6. Counterpart of an Agreement: Department of Chemistry, University of Cambridge Name of an Agreement: AGREEMENT ON ACADEMIC EXCHANGE BETWEEN THE WORLD PREIER INTERNATIONAL RESEARCH CENTER ADVANCED INSTITUTE FOR MATERIALS RESEARCH (WPI-AIMR) TOHOKU UNIVERSITY, JAPAN AND DEPARTMENT OF CHWMISTRY UNIVERSITY OF CAMBRIDGE, UNITED KINGDOM

Dates of an Agreement: January 18, 2011

Summary of an Agreement:

- Promotion of joint research and educational activities
- Invitation to short-term visits of researchers for academic activities
- Exchange of information and pertinent publication in fields of interest to both universities
- Exchange of faculty members, researchers and students for study and research
- 7. **Counterpart of an Agreement:** The Particulate Fluids Processing Centre (PFPC), The University of Melbourne

Name of an Agreement: AGREEMENT ON ACADEMIC EXCHANGE BETWEEN WORLD PREMIER INTERNATIONAL RESEARCH CENTER – ADVANCED INSTITUTE FOR MATERIALS RESEARCH (WPI-AIMR), TOHOKU UNIVERSITY, JAPAN AND THE PARTICULATE FLUIDS PROCESSING CENTRE (PFPC), THE UNIVERSITY OF MELBOURNE, AUSTRALIA

Dates of an Agreement: October 26, 2011

Summary of an Agreement:

- Promotion of joint research and educational activities
- Invitation to short-term visits of researchers for academic activities
- Exchange of information and pertinent publication in fields of interest to both universities
- Exchange of faculty members, researchers and students for study and research
- 8. **Counterpart of an Agreement:** Fraunhofer Institute for Electronic Nano Systems (ENAS) **Name of an Agreement:** MEMORANDUM OF UNDERSTANDING

ON ACADEMIC EXCHANGE BETWEEN THE WORLD PREMIER INTERNATIONAL RESEARCH CENTER

ADVANCED INSTITUTE FOR MATERIALS RESEARCH (WPI-AIMR) TOHOKU UNIVERSITY, JAPAN

AND FRAUNHOFER GESELLSCHAFT ZUR FÖRDERUNG DER ANGEWANDTEN FORSCHUNG e.V. for its Fraunhofer institute for Electronic Nano Systems (enas), Germany

Dates of an Agreement: November 8, 2011

Summary of an Agreement:

- Promotion of joint research and educational activities
- Invitation to short-term visits of researchers for academic activities
- Exchange of information and pertinent publication in fields of interest to both universities

- Exchange of faculty members, researchers and students for study and research
- Study on the establishment of a Fraunhofer Project Center
- 9. **Counterpart of an Agreement:** Institute for Pure and Applied Mathematics (IPAM), University of California, Los Angeles (UCLA)

Name of an Agreement: MEMORANDUM OF UNDERSTANDING THE REGENTS OF THE UNIVERSITY OF CALIFORNIA, ON BEHALF OF ITS LOS ANGELES CAMPUS, USA AND THE ADVANCED INSTITUTE FOR MATERIALS RESEARCH (AIMR) TOHOKU UNIVERSITY, JAPAN

Dates of an Agreement: August 2, 2012

Summary of an Agreement:

- Visits and informal exchanges of faculty, scholars and administrators in specific areas of education, research and outreach
- Organize joint conferences, or other scientific meetings on subjects of mutual interest
- Explore the possibilities for developing joint research programs and collaborations
- Other exchange and cooperation programs to which both parties agree
- 10. **Counterpart of an Agreement:** The Department of Pure Mathematics and Mathematical Statistics (DPMMS), University of Cambridge

Name of an Agreement: AGREEMENT ON ACADEMIC EXCHANGE BETWEEN ADVANCED INSTITUTE FOR MATERIALS RESEARCH (AIMR) TOHOKU UNIVERSITY, JAPAN AND DEPARTMENT OF PURE MATHEMATICS AND MATHEMATICAL STATISTICS, UNIVERSITY OF CAMBRIDGE, UNITED KINGDOM

Dates of an Agreement: April 8, 2013

Summary of an Agreement:

To promote cooperation in joint research and educational activities

11. Counterpart of an Agreement: Fraunhofer Institute for Algorithms and Scientific

Computing SCAI, Institute for Mechanics of Materials IWM

Name of an Agreement: Memorandum of Understanding BETWEEN

Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V., Fraunhofer Institute for Algorithms and Scientific Computing SCAI AND Advanced Institute for Materials Research (AIMR), Tohoku University

Dates of an Agreement: August 6, 2013

Summary of an Agreement:

- · Cooperation in technical and scientific issues
- Exchange of technical and scientific information
- Exchange of professionals
- · Cooperation in developing new projects
- Exchange of R&D market information
- 12. Counterpart of an Agreement: POLITECNICO DI TORINO

Name of an Agreement: AGREEMENT ON ACADEMIC EXCHANGE BETWEEN TOHOKU

UNIVERSITY, JAPAN AND POLITECNICO DI TORINO, ITALY

Dates of an Agreement: November 24, 2010

Summary of an Agreement:

- Promotion of joint research and educational activities
- Invitation to short-term visits of researchers for academic activities
- Exchange of information and pertinent publication in fields of interest to both universities
- Exchange of faculty members, researchers and students for study and research
- 13. Counterpart of an Agreement: Chemnitz University of Technology

Name of an Agreement: AGREEMENT ON ACADEMIC EXCHANGE BETWEEN TOHOKU UNIVERSITY, JAPAN AND CHEMNITZ UNIVERSITY OF TECHNOLOGY, GERMANY

UNIVERSITY, JAPAN AND CHEMINITE UNIVERSITY OF TECHNOLOGY, GET

Dates of an Agreement: October 31, 2013

Summary of an Agreement:

- Promotion of joint research and educational activities
- Invitation to short-term visits of researchers for academic activities
- Exchange of information and pertinent publication in fields of interest to both universities
- Exchange of faculty members, researchers and students for study and research
- **14. Counterpart of an Agreement:** INSTITUTE OF CHEMISTRY, CHINESE ACADEMY OF SCIENCE

Name of an Agreement: AGREEMENT FOR JOINT OPERATION OF THE AIMR SATELLITE

FACILITY AT INSTITUTE OF CHEMISTRY, CHINESE ACADEMY OF SCIENCE

Dates of an Agreement: July 31, 2012

Summary of an Agreement: Promotion of AIMR Satellite Operations at ICCAS

15. Counterpart of an Agreement: California Nanosystems Institute, University of California, Santa Barbara

Name of an Agreement: AGREEMENT FOR AN ADVANCED INSTITUTE FOR MATERIALS RESEARCH (AIMR) JOINT SATELLITE RESEARCH CENTER AT CALIFORNIA NANOSYSTEMS INSTITUTE (CNSI), UNIVERSITY OF CALIFORNIA, SANTA BARBARA

Dates of an Agreement: July 2, 2012

Summary of an Agreement: Promotion of AIMR Satellite Operations at CNSI

16. Counterpart of an Agreement: Department of Pure Mathematics and Mathematical Statistics, University of Cambridge (DPMMS)

Name of an Agreement: AGREEMENT FOR ADVANCED INSTITUTE FOR MATERIALS RESEARCH (AIMR) JOINT CENTRE AT THE DEPARTMENT OF PURE MATHEMATICS AND MATHEMATICAL STATISTICS, UNIVERSITY OF CAMBRIDGE

Dates of an Agreement: October 1, 2013

Summary of an Agreement:

To operate the AIMR Joint Centre as AIMR satellite facility at DPMMS

17. Counterpart of an Agreement: Materials Science & Metallurgy, University of Cambridge (MSM)

Name of an Agreement: AGREEMENT FOR ADVANCED INSTITUTE FOR MATERIALS RESEARCH (AIMR) JOINT CENTRE AT THE DEPARTMENT OF MATERIALS SCIENCE & METALLURGY, UNIVERSITY OF CAMBRIDGE

Dates of an Agreement: November 1, 2013

Summary of an Agreement:

To operate the AIMR Joint Centre as AIMR satellite facility at MSM

18. Counterpart of an Agreement: Department of Chemistry, University of Cambridge Name of an Agreement: AGREEMENT FOR ADVANCED INSTITUTE FOR MATERIALS RESEARCH (AIMR) JOINT CENTRE AT THE DEPARTMENT OF CHEMISTRY, UNIVERSITY OF CAMBRIDGE

Dates of an Agreement: December 1, 2013

Summary of an Agreement:

To operate the AIMR Joint Centre as AIMR satellite facility at Department of Chemistry

19. Counterpart of an Agreement: The University of Chicago

Name of an Agreement: MEMORANDUM OF UNDERSTANDING REGARDING

THE PROPOSED JOINT RESEARCH CENTER BETWEEN AIMR AND THE UNIVERSITY OF CHICAGO

Dates of an Agreement: April 16, 2014

Summary of an Agreement:

To operate the U.CHICAGO/AIMR Joint Research Centre at both institutes

6. Holding international research meetings

*Give up to twenty examples of the most representative ones of international research conferences or symposiums held between FY2007-2013 using the table below.

Date	Meeting title and Place held	Number of participants	
February 16 th – 19 th , The AIMR International Symposium 2014 (AMIS2 2014 (Sendai, Japan)		236	
November 22 nd , 2013	·		
November 21 st , 2013	Tohoku University Day (London, UK)	77	
November 20 th , 2013	WPI-AIMR/Cambridge Workshops and Discussions on "Hierarchical materials for green energy" (Cambridge, UK)	30	
October 24 th , 2013	1 st University of Bordeaux/Tohoku University Joint Symposium (Sendai, Japan)	100	
September 28 th -30 th , 2013	International Symposium for the 70th Anniversary of the Tohoku Branch Chemical Society of Japan (Sendai, Japan)	1000	
May 12 th -16 th , 2013	17th International Symposium on Intercalation Compounds (Sendai, Japan)	200	
February 22 nd , 2013			
February 22 nd , 2013	WPI-AIMR and Fraunhofer ENAS Joint Workshop on Micro Integrated Devices (Sendai, Japan)	60	
February 18 th -21 st , 2013 The AIMR International Symposium 2013 (AMIS2013) (Sendai, Japan)		240	
November 9 th -10 th , 2012	Sendai Symposium on Analytical Sciences 2012 (Sendai, Japan)	70	
May 19 th -20 th , 2012	AIMR-PFPC Joint Workshop (Sendai, Japan)	40	
May 13 th -18 th , 2012	International Association of Colloid and Interface Scientist, Conference (IACIS2012) (Sendai, Japan)	1000	
February 21 st -23 rd , 2012	-		

January 9 th -13 th , 2012	UCSB ICMR/CNSI and Tohoku University WPI-AIMR Joint Workshop on Materials Research (Santa Barbara, USA)	34
June 12 th -14 th , 2011	WPI-AIMR Cambridge Symposium (Cambridge, UK)	15
February 22 nd -24 th , 2011	The 2011 WPI-AIMR Annual Workshop (Sendai, Japan)	216
March 25 th -27 th , 2010	The 2010 WPI-AIMR Annual Workshop (Sendai, Japan)	192
August 25 th -28 th , 2009	WPI-Europe Workshop (Grenoble, France)	80
March 1 st -6 th , 2009	The 2009 WPI-AIMR Annual Workshop (Zao, Miyagi, Japan)	180

World Premier International Research Center Initiative (WPI)

1. Host institution's commitment

1-1. Contributions from host institution

(1) Fund, Personnel

(2007-2014)									
<fund> (million yen)</fund>									
Fiscal Year	2007	2008	2009	2010	2011	2012	2013	2014	Total
Personnel - Faculty members (including researchers)	11	164	243	24	75	257	242	197	1,213
Full-time Concurrent - Postdocs - RA etc. - Research	9	94	130	19	3	188	177	125	736 9
support staffs - Administrative		1	24				1		26
staffs	2	69	89	5	72	69	64	72	442
Project activities	5	101	105	116	122	53	3	24	529
Travel	0	8	7	1	0	8	1	0	25
Equipment	0	932	161	0	61	30	39	30	1,253
Research projects	350	599	204	193	30	18	38	31	1,463
Total	366	1,804	720	334	288	366	323	282	4,483
<personnel></personnel>						(person)			
Fiscal Year	2007	2008	2009	2010	2011	2012	2013	2014	Total
Personnel - Faculty members (including researchers)	2	15	14	16	3	18	19	18	105
Full-time Concurrent - Postdocs - RA etc.	2	13 2	12 2	15 1	3	16 2	17 2	16 2	92 13
- Research support staffs		2	12				1		15
- Administrative staffs	1 (0)	12 (11)	24(11)	12 (12)	17 (16)	10 (10)	10 (10)	10 (10)	96 (80)

^{*} Regarding "Fund" entry, describe with reference to the items in the Progress Report(実績報告書,Jisseki-hokoku-sho)based on Article 12 of the Grant Guidelines(交付要綱,Kofu-yoko).

^{*} Don't include competitive funding obtained by researchers (used as research project funding)

^{*} Under "Personnel", enter the number of full-time administrative staff within the parenthesis.

(2) Provision of land and/or building(s), lab space, etc.

In FY2008, the host institution, Tohoku University, renovated an existing 2,221 m² building in the Katahira Campus and offered it to the Center (AIMR) as a research facility (present name: ANNEX Building). Subsequently, the host institution built a new WPI Building (first term construction: 3,650 m²) in FY2007 and a WPI Building (second term construction: 3,287 m²) in FY2008, completing the present "Integration Laboratory Building." Additionally, the host institution built the new AIMR Main Building (8,161 m²) in FY2011 with matching funds from the Facility Maintenance Expense Subsidy from MEXT, and currently offers about 17,300 m² total of the three buildings to the Center for research space. Furthermore, the host institution has covered the necessary expenses for setting up common facilities required for research and refining research space. As a result, large-scale infrastructures have been constructed. These include helium-collecting plumbing for recycling that covers the whole Integration Laboratory Building, completed in FY2009; an energy monitoring system set up in FY2012; a centralized plumbing facility providing special gases, constructed in the AIMR Main Building in FY2013; and helium-collecting plumbing covering the Annex Building, completed in FY2013. Besides these resources from the host institution, 50% of indirect costs of the external funds obtained by researchers belonging to the Center have been provided to the Center.

1-2. System under which the center's director is able to make substantive personnel and budget allocation decisions

To secure the independence of the Center's administration, the host institution retains authority solely for extremely important items. Other items, such as personnel affairs and budget execution, are essentially determined by the Center Director. In other words, with regard to personnel affairs, the host institution only retains authority over the appointment and dismissal of the Center Director. Other personnel affairs within the Center, including the employment of PIs, are at the discretion of the Center Director. The WPI grant allotted to the Center has been entirely turned over to the Center, and the Center Director can execute the budget that includes not only the WPI grant, but also the budget allocated by the host institution depending on the judgment by the Center. The Center Director is given authority to make the final decision alone.

1-3. Support for the center director in coordinating with other departments at host institution when recruiting researchers, while giving reasonable regard to the educational and research activities of those departments

Before the establishment of the Center, the host institution had already set up a meeting comprised of the heads of the related departments and the President of Tohoku University as the chairperson, and adjusted opinions. In the meeting, the status and terms of office of the researchers placed at the Center from the host institution, research space, administrative support, and the problem of education and research activities at the past position were discussed, and the support system for the Center Director was arranged. Since June 2010, the AIMR In-house Council, consisting of heads of related departments and institutes and taking over the function of the above meeting, has been organized and acts as adviser to the Center Director from the standpoint of the entire university.

- 1-4. Revamping host institution's internal systems to allow introducing of new management methods
 - (e.g., English-language environment, merit-based pay, cross appointment, top-down decision making unfettered by conventional modes of operation)
 - (1) Top-down decision-making system: AIMR established the "International Advisory Board," including Nobel Prize laureates as members; and the "External Advisory Board" comprised of outside professionals, which hold regular meetings and advise the Center Director to support top-down decision-making by the Center Director.
 - (2) English-language environment: Since the establishment of the Center, the host institution has preferentially assigned staff members, most of whom not only provide bilingual administration services in English and Japanese, but are also permanent staff skilled in accounting, personnel affairs, and research support in the host institution, to the Center's Administrative Division. In addition to this, the Center employed staff members with skill in safety and health management or information communication management and English from outside the university. Consequently, the Center succeeded in organizing the Administrative Division, where 90% or more of staff can provide services in English. The host institution plans to transform the Center's Administrative Division, which has accumulated the know-how and skill for English services, into the international administrative office and Research Reception Center of the Organization for Advanced Studies, (established in FY2014) and have them lead the internationalization of the host institution.
 - (3) Merit-based salary system: The host institution leaves decisions about special allowances for the researchers and decisions on salary amounts for the annual salary scheme to the Center Director. Since the establishment of the Center, a monthly allowance (¥100,000; PI allowance) from the host institution has been paid to full-time PIs who are participating in the Center. Merit-based wage depending on the result of a performance evaluation every fiscal year (four levels: ¥80,000, ¥60,000, ¥40,000, and ¥20,000 per month) has been given to excellent researchers; and an affiliated PI allowance (¥100,000 per month) has been paid for affiliated PIs who belong to other departments in the host institution. All special allowances are based on approval by the Center Director.
 - (4) Top management: The host institution prepared the system to respond rapidly to requests from the Center Director regarding revision, improvement, or adjustment of the host institution's systems. In FY2012, the "Project Team (PT) for Promotion of World Class Research" and the "PT for Promotion of Global Strategy" were established under the Executive Vice President of the host institution. These PTs have often taken up the achievement and future advancement of the WPI Program as subjects for discussion. Such further reinforcement of in-house cooperation and support ensures smooth conduct of the top management by the Center Director.
 - (5) System of administration reform: The host institution is conducting various support, such as revision of the existent rules of the host institution, in order to spread the system reform and internationalization tackled by the Center into the whole institution. In particular, the host institution gave notice through the headquarters to the whole institution in FY2013 with respect to revision of the contract procedure for the employment of overseas researchers based on joint appointment, and directly sending airline tickets to foreign researchers for invitation. Furthermore, the accumulated examples of the documents for the bilingual administrative services have been summarized in the books "Examples of English e-mails and letters for administrative staff" and "Examples of English conversation," and will be distributed to all administrative staff in the host

institution in FY2014.

1-5. Accommodation of center's requirements for infrastructural support
Utilities and other infrastructure support provided by host institution.

(*In addition to listed in the item 1. Contributions from host institution)

The host institution completed the AIMR Main Building in FY2011 as the core facility of the Center's activities, gathering all researchers under one roof. On this occasion, the host institution afforded Center's researchers support to use the facilities of other departments in the Katahira Campus, such as their library, materials analysis facility, and liquid nitrogen supply facility. In addition, the host institution built the new Katahira Kitamon Commons near the AIMR Main Building in FY2012, which possesses lodging for researchers from abroad, assuring space for researchers whom the Center invites.

1-6. Support for other types of assistance

Other than those above, the host institution stipulated support to the Center in both the first and second interim plans of the "Mid-term Plan" of Tohoku University. The host institution will provide the Center full support as a "special ward, Organization for Advanced Studies," and will utilize the Center as the core institute for both education and research based on scientific achievements, increase of its international presence, system reform, and reform of the sense of the faculties and administrative staff (in particular, administration for international services), and challenge new orientation research, achieved by the Center since its establishment in FY2007, aiming to develop into a world-class institute.

2. **Tohoku University Mid-Term Plan**

Approved by Minister of Education, Culture, Sports, Science and Technology on March 31, 2010 Revisions approved by Minister of Education, Culture, Sports, Science and Technology on March 31, 2011 Revisions approved by Minister of Education, Culture, Sports, Science and Technology on March 30, 2012 Revisions approved by Minister of Education, Culture, Sports, Science and Technology on March 29, 2013 Revisions approved by Minister of Education, Culture, Sports, Science and Technology on March 31, 2014

I. Measures which should be taken for achieving goals related to increasing the quality of university education, research, etc.

1.

1. Measures for achieving education goals
(1) Measures for achieving goals related to education programs and education outcomes, etc.
①-1 Re-development of Tohoku University's unique liberal arts education curriculum
☐ Establish Tohoku University's unique liberal arts education curriculum to enhance the human capacities of students, broaden their global perspectives, establish the foundation of professional education, and conduct interdisciplinary research at graduate schools.
2-1 Enhancement of undergraduate professional education
☐ Enhance the curriculum of undergraduate professional education to ensure that students are equipped with the ability to understand and apply in their fields of specialty, which serve as the basis for the expertise and internationalism necessary for social contributions, and to ensure that students are equipped with the basic expertise and execution abilities to make a smooth transition to high-level professional education upon enrollment in graduate school.
2-2 Re-development of graduate school education curriculum
□ Develop a curriculum that is suitable for a high-level graduate school education built upon liberal arts education and foundational specialized courses.
 2-3 Rigorous and appropriate evaluation of students' academic performance Conduct rigorous and appropriate evaluation of students' academic performance that guarantees high standards of education programs. 2-4 Development of skilled researchers in interdisciplinary fields
Conduct education programs for fostering skilled researchers in interdisciplinary fields in cooperation with the Institute for International Advanced Research and Education, Advanced Institute for Materials Research (AIMR), and Global COE Program.
2–5 Development of world-leading personnel with PhDs
☐ In the area of spintronics, establish an international cooperative graduate school by FY2015 as part of an education program to foster world-leading personnel with PhDs through collaborations between Tohoku

②-6 Development of personnel in fields with particularly high societal demands
☐ Implement education programs for fostering highly specialized professionals in a planned manner, in order to meet the expectations for fostering highly specialized professionals in fields with particularly high societal demands.
③-1 Development of international networks, promotion of students' overseas studies, increases in number of accepted international students, etc.
☐ Conduct programs such as study abroad programs and overseas internship programs by building international networks with international-standard universities and organizations.
☐ Further develop an environment for accepting international students to increase the number of accepted international students.
4-1 Increases in student recruitment capabilities
 □ Carry out public relations activities to motivate students to enroll at Tohoku University, including creating an easy-to-understand website and holding informational sessions, open campuses, and travelling lectures. ④-2 Improvement of methods for selecting enrolling students who conform to the admissions policy
☐ Continuously check and improve methods for selecting enrolling students in order to ensure that students conform to the admissions policy.
(2) Measures for achieving goals related to the system for implementing education, etc.
①-1 Establishment and enhancement of system for implementing liberal arts education
☐ Establish core education and research organizations for strengthening liberal arts education through a whole-of-university approach.
①-2 Establishment and enhancement of system for implementing undergraduate professional education and graduate school education
☐ To ensure faculty diversity, increase the number of non-Japanese faculty and promote appropriate faculty assignments that take into consideration factors such as age distribution, gender balance, and experience. ①-3 Expansion of system of e-learning education
☐ Expand system of e-learning education for offering efficient and effective education.
①-4 Promotion of measures for increasing the quality of education
☐ To increase the quality of education, promote education improvement activities, including continuous reviews of the implementation system and method of education. In doing so, also undertake efforts to achieve a proper enrollment quota for the Undergraduate School of Dentistry.
(3) Measures for achieving goals related to supports for students
①-1 Enhancement of learning supports
☐ Enhance learning support initiatives.
①-2 Enrichment of extracurricular activities, etc.
☐ Enrich extracurricular activities, etc. to improve human relations skills and foster social skills.
①-3 Promotion of career supports
☐ Promote career support initiatives.

2. Measures for achieving research goals

(1) Measures for achieving goals related to the standards of research and research outcomes, etc.
①-1 Enhancement of basic research based on long-term perspective
☐ Support and promote research that reflects the free thinking and creativity of departments and researchers in light of the importance of basic research and the inseparability of basic research and applied research.
☐ Further improve the operations of joint usage/research centers, in order to go beyond university boundaries and execute missions as core institutions in related research areas that are open to the entire country.
☐ Further improve the operations of institutes to allow them to fully exercise their functions while adapting to scholarly research trends and changes in the economy and society, and to execute missions as core research centers of scholarly research that maintain a high research standard.
①-2 Promotion of strategic research that addresses social issues
 □ Promote strategic research that addresses social issues by integrating social needs and Tohoku University's diverse research seeds. Promote research that will lead the way towards the reconstruction of the areas affected by the Great East Japan Earthquake and regional revitalization. ①-3 Development of world-leading scientific research on priority areas
Strengthen and support AIMR, which was launched with the adoption by the World Premier International
Research Center Initiative (WPI), to develop AIMR into a world-leading international research network hub.
☐ Promote international project research and joint programs as a core research center, including the adoption of the Global COE Program.
2–1 Drive forward innovative research of the Institute for International Advanced Research and Education, etc.
Promote innovative research by making use of the Institute for International Advanced Research and
Education, AIMR, Graduate School of Biomedical Engineering, among other institutes of Tohoku University. 2-2 Promotion of translational research (research that bridges basic research with clinical applications)
☐ To promote translational research (research that bridges basic research with clinical applications), make enhancements to the Innovation of New Biomedical Engineering Center and build a system of education for fostering personnel who will promote translational research.
 ③-1 Promotion of international joint research through building global networks □ Promote international joint research through global academic networks with international-standard universities and research institutions. In particular, in the area of spintronics, invite world-leading non-Japanese researchers from overseas universities and other institutions and promote cutting-edge international joint research.
 (2) Measures for achieving goals related to the framework of research implementation, etc. ①-1 Strengthening of strategic research support functions □ Strengthen strategic research support functions that integrate social needs and Tohoku University's diverse research seeds.

3. Transition in the number of female researchers

Enter the number and percentage of female researchers in the top of each space from 2010 to 2013 and the total number of all the researchers in the bottom.

(Person)

		FY2010	FY2011	FY2012	FY2013	Final goal
	Daga a mahama	14, 10%	11, 8%	15, 9%	16, 9%	22, 15%
F	Researchers	136	131	165	170	146
	Principal	2, 6%	2, 6%	2, 6%	2, 6%	2, 6%
	investigators	33	32	32	31	33
	Other	12, 12%	9, 9%	13, 10%	14, 10%	20, 18%
	researchers	103	99	133	139	113