

World Premier International Research Center Initiative (WPI)

Executive Summary (for Final Evaluation)

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

About filling out this form:

This summary is to be based on the Center's Progress Report and Progress Plan, with reference to the following items, prepare the summary within a space of **up to 6 pages**.

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 structures producing such 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 2,609 papers including 73 papers appearing in *Science, Nature, and Nature's sister journals,* and received internationally-acclaimed awards such as *the American Physical Society's Oliver E. Buckley Condensed Matter Prize, Humboldt Research Award, IEEE David Sarnoff Award, and IEEE Andrew S. Grove Award.* It was concluded by the WPI Program Committee that AIMR has already achieved "World Premier Status."

AIMR's challenge attracts talented researchers from around the world, making it an international research center. Around 50% of researchers or more are from overseas. The official language is English and research support is substantial. Regarding international cooperation, AIMR established joint laboratories in the University of Cambridge, the University of California, Santa Barbara, and the University of Chicago, 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 a hub of global brain circulation.

On system reform, AIMR has achieved independence from the university and top-down decision-making by the Center Director. Besides English services, thorough support for researchers allows them to start research almost immediately. These efforts have created ripple 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 and structures producing such 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. Motoko 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 *Physical Review Letters* 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.”** Such 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. Based on these facts the WPI Program Committee concluded that AIMR has already achieved “World Premier Status” in *FY2014 Follow-up Report*.

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 eight and a half years following the Center’s establishment, the number of publications has increased steadily. AIMR researchers have published 2,609 papers, with 73 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*, *the IEEE Andrew S. Grove 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 2.1-3.4 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 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; the University of Cambridge, the University of California, Santa Barbara (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. In recent years, AIMR strengthened the relationship with the University of Chicago; AIMR and the University of Chicago signed the agreement in FY2014 and established a joint laboratory in FY2015. 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, 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 in the Administrative Division, thorough support for researchers allows them to start research immediately after arrival. These efforts have created ripple effects through the host institution. Tohoku University has established 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 AIMR's experiences have become a driving 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 (specially-appointed associate 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 has established "Graduate Program in Spintronics (GP-Spin)," where AIMR researchers are playing a central role and world-leading researchers and graduate students are gathering.

B. Progress Plan

1. Mid- to Long-term Research Objectives and Strategies Based on the Center's Research Results to Date

AIMR's research accomplishments have been evaluated as "world-leading" every year since its establishment by the WPI Program Committee and international scientific communities. AIMR clarified its identity as "discovering common elements and universal principles among different material fields and creating new materials science which can predict new functions and structures producing such functions," by injecting mathematical viewpoints. Concrete evidence such as the publication of papers in high impact journals, receipt of internationally-acclaimed academic awards, and a world-leading research environment and support system indicates that AIMR has already achieved "World Premier Status."

After the termination of the ten-year support by WPI program, AIMR will maintain its organization and management system, flexibly and quickly implementing strategy for present needs, as well as an engaging research environment with excellent researchers from around the world. Under such excellent environment and system, AIMR will deepen and mature the mathematics-materials science collaboration that has been developed over the past four years, making it a standard aspect of materials science in the 21st century. Specifically, results are already emerging in "**Spin-centered materials science**" and "**Design of hierarchical structure based on theoretical prediction.**" These will be future priority areas.

The interaction of mathematics with other fields was regarded as the most important theme in the U.S. Odom Report and Brown Report and the OECD Report on Mathematics in Industry. In line with this global movement, AIMR has begun mathematics-materials science collaboration at the institutional level; a world first. AIMR has a great chance to set a global trend and become a world leader. Another recent global trend is big data analysis by highly functional numerical calculation technology. AIMR can also play a central role here as its mathematics-materials science collaboration aims to discover common principles hidden behind the complicated structures, which is suited to this area. Based on these measures, as a long-term objective, AIMR will become a world leader in materials science with flexible and quick strategy in line with present needs, and contribute to society by creating revolutionary functional materials based on the new materials science born at AIMR.

2. Management System of the Research Organization

The existing structure of five research groups is maintained, "Materials Physics," "Non-equilibrium Materials," "Soft Materials," "Device/System," and "Mathematical Science." Center Director Kotani will continue the flexible and quick personnel management based on top-down decision-making and, using the "joint appointment system" that AIMR institutionalized, increase the mobility of human resources within the university and among research groups inside and outside Japan. The Administrative Division of AIMR will be transformed into the international administrative office and the research reception center in the Organization for Advanced Studies. The Know-how accumulated at AIMR will be utilized for

support systems and services for inviting overseas researchers at the Organization for Advanced Studies.

Regarding international expansion, AIMR will maintain the international partnership with five institutions, the University of Cambridge, the University of California, Santa Barbara (including the partnership with CNSI and IPAM, UCLA), Beijing (Tsinghua University and Chinese Academy of Sciences), Chemnitz University of Technology (Fraunhofer ENAS) and the University of Chicago. The superiority of AIMR in such international partnerships is realized in the mathematics-materials science collaboration first pioneered by AIMR. The importance of cooperation between various fields and mathematics, which serves as the bedrock for innovation, has been repeatedly noted; and the global trend of mathematics cooperating with other fields is clearly progressing. In this movement, bringing the mathematics-materials science collaboration pioneered by AIMR into the global arena is a response to global demands. AIMR has started a global trend and is becoming a world leader.

3. Center's Position within the Host Institution, and Measures Taken by Host Institution to Provide Resources to the Center

Promotion of AIMR is one of the most important missions in Tohoku University's mid-term plan. Even after WPI support ends, Tohoku University has decided to sustain AIMR as a world top level research center leading the university's world-class research and internationalization. In FY2014, Tohoku University established the "Organization for Advanced Studies" under the direct control of the President and made AIMR its first institute. The Administrative Division of AIMR and its accumulated know-how of international work will become the new organization's international administrative office and the research reception center. It will lead efforts to advance internationalization across the university. "Tohoku Forum for Creativity" established in FY2013 as a visiting theoretical research center that invites global authorities has also been part of the Organization for Advanced Studies. AIMR will form the core for reinforcing research capability, internationalization, and system reform in close association with the forum.

Besides existing permanent staff (16 researchers and 10 administrative staff), President Satomi promised to add 10 tenure positions to maintain AIMR's activities. The financial resource from the host institution will be used mainly to start the laboratories of the new tenured researchers and keep the young researchers of the Mathematical Science Group and staff of the international administrative office. Part of the resource will also be used to maintain cooperative relationship with the overseas satellites as mentioned above. It is necessary to maintain research and international activities by keeping at least two thirds of the present scale (especially the number of young researchers) of the Center in order for AIMR to keep a position as the world leader to create new materials science based on mathematics-materials science collaboration. We will make maximum effort to keep young experimental researchers (assistant professors and postdoctoral researchers) by using external sources.

World Premier International Research Center Initiative (WPI) Progress Report of the WPI Center (for Final Evaluation)

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| 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 2016) 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 1-1~7], 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, project funding, project expenditures, and WPI grant expenditures.

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 and structures producing such 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 progress in 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. AIMR cleared the two-year careful observation by making "remarkable progress beyond expectation"

within two years, 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. Collaboration like this at an institutional level is unprecedented, attracting great interest from the materials science and mathematics communities.

Since its establishment, AIMR has pursued world-leading research 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 2015, AIMR researchers have published 2,609 papers, including 73 papers appeared 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*, *the IEEE David Sarnoff Award*, and *the IEEE Andrew S. Grove Award* led to the conclusion by the WPI Program Committee that AIMR has already achieved "World Premier Status" as shown in *FY 2014 Follow-up Report*.

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. 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, the University of California, Santa Barbara, and the University of Chicago 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 functions as a hub for global brain circulation.

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 2016. 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 2-1, 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_6Ca 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 $BaFe_2As_2$, 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 (see Appendix 3, Paper no. 1). An epoch-making discovery, rejuvenation by thermal treatment of metallic glasses, has also been achieved and the mechanism of the phenomenon at atomic level is under investigation. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 11-14 Published in **Physical Review Letters, Nature Materials, Nature**)

[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] 15-17 Published in **Nature Materials, 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 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, 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] 18-20 Published in **Nature Materials, Nature Communications**)

***[8] Molecular superconductors**

At AIMR, there exist two laboratories holding the world records of critical temperature for superconductors in molecular crystal systems (33 kelvin under atmospheric pressure and 38 kelvin under a high pressure) and world's cutting-edge research has been carried out in this field. Recently, these laboratories obtained interesting experimental results which will advance the understanding of molecular superconductors. One is the discovery of dome-like variation of the critical temperature with the density of cesium fulleride (Cs_3C_{60}) molecules. Researchers also identified a new metallic phase, which they termed "a Jahn-Teller metal." The other is the discovery of superconductivity of BaC_6 which has not been discovered for many years though it has been theoretically predicted. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 21, 22 Published in **Science Advances, 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. Generally, 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 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] 23 Published in **Physical Chemistry Chemical Physics**)

***[10] Molecular motors**

Recently, interesting discoveries have been achieved in the field of molecular motors at AIMR. Miniature chemical reactors which can transport things like drugs in the body or which enable biosensing are expected to be developed. However, limitation of their further miniaturization of the reactors prevents them from being directly implanted into the body. AIMR researchers developed a much smaller system that uses a natural motor protein, Kinesin-1, to transport cargo along a track made of carbon nanotubes. In the other research, AIMR researchers succeeded in synthesizing a carbonaceous molecular bearing comprising a belt-persistent tubular molecule and a fullerene molecule. Furthermore, they theoretically investigated the rotational motion of the molecular bearing and revealed that the motions comprises two distinct motions, precession and spin. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 24, 25 Published in **Nano Letters, Chemical 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] Three-dimensional nanoporous graphene**

Graphene is a two-dimensional (2D) sheet material showing high electric conductivity and having potential for replacing silicon or noble metals in the future. Graphene is attracting much interest of researchers of all over the world especially after Andre K. Geim and Konstantin Novoselov were awarded Nobel Prize in physics in 2010. The perfect, honeycomb-like bonding inside a sheet of graphene allows charge carriers to move through the material as massless particles called Dirac fermions. This phenomenon gives graphene intrinsically higher electron mobility than any other known material. So far, many researchers tried to create three-dimensional (3D) material of graphene for further applications, but nobody has never succeeded in obtaining 3D graphene preserving high mobility. AIMR's research team consisting of researchers from different laboratories has succeeded in producing 3D nanoporous graphene that preserves the massless Dirac fermions of 2D systems showing high mobility. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 30 Published in **Angewandte Chemie International Edition**)

***[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. Researchers from AIMR discovered an excellent ion conductivity of a sodium-based complex hydride, $\text{Na}_2\text{B}_{10}\text{H}_{10}$, highly promising for use as a solid electrolyte in rechargeable batteries. (Papers underscoring the research achievement above and their brief account: [Appendix 2-1] 33, 34 Published in **Nanotechnology, Advanced Materials**)

***[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 (C_{60}) 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** in each year from 2007 to 2015 are 0, 2, 5, 5, 10, 8, 17, 11, and 15, respectively.

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 2-2, 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, more than 2.1 billion yen has been accumulated after the second year. 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**) and conducted their projects until the end of FY2013. Prof. Hiroyuki Isobe (PI) and Prof. Eiji Saitoh (PI) won the the Exploratory Research for Advanced Technology (**ERATO**) research funding program, starting the project from FY2013 and FY2014, respectively, in AIMR's buildings. There are other several projects which were or still are being carried out by AIMR PIs. These include Gran-in-Aid for Scientific Research Scientific Research **S**, the Strategic Basic Research Programs (**CREST**), Green Network of Excellence (**GRENE**), projects supported by New Energy and Industrial Technology Development Organization (**NEDO**), and projects provided by Cross-ministerial Strategic Innovation Promotion Program (**SIP**). 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 2,609 papers from October 2007 through December 2015. Among those, if we especially focus on the papers produced by international collaboration, 1,130 papers (43.3%) were results of international collaboration. Aside from the fusion research inside the Center, AIMR researchers have carried out numerous joint research projects with other institutions, in particular, institutions 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 2-3, list the 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, the IEEE David Sarnoff Award, and the IEEE Andrew S. Grove Award. Researchers have also given many invited 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 nine 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 nine 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, a consortium consisting of more than 70 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;" FY2013-2021 (Research Leader: PI

Prof. Tomokazu Matsue)

- Cross-ministerial Strategic Innovation Promotion Program (SIP): Prof. Yasumasa Nishiura (PI), Prof. Kazue Kurihara (PI) and Prof. Tadafumi Adschiri (PI) are participating in “Structural Materials for Innovation,” “Innovative Combustion Technology” and “Innovative Design and Production Technology,” respectively.

Intellectual properties (IPs):

- Terunobu Miyazaki and Shigemi Mizukami “Magneto-resistive element and magnetic memory” US Patent, US8520433 Apr. 27, 2013.
- Seiji Samukawa “Low dielectric constant insulating film and method for forming the same” US Patent, US8,828,886 Sept. 9, 2014.
- 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
- Shin-ichi Orimo “SOLID-STATE BATTERY” Filing date: August 27, 2017 International Appl. No.: PCT/JP2014/072438 International unexamined patent publication (Kokai) No.: WO/2015/030052 (March 5, 2015)
- 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 180 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. Based on this new technology, a consortium comprising more than 70 companies has been established and research and development for the practical use are proceeding.

Prof. Shigemi Mizukami, Prof. Emeritus Terunobu Miyazaki and co-workers (Mizukami laboratory since FY2013) collaborated with Toshiba Corporation for new materials development to realize nonvolatile MRAM (magnetoresistive random access memory), where T. Miyazaki is a pioneer 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 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 almost 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 was installed in Tohoku University in FY2014.

Prof. Shin-ichi Orimo and co-workers are pursuing the research and development of new energy 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 development of mass production technology for LiBH₄-based solid electrolytes. Furthermore, they established an Industrial-Academic Partnership Project in AIMR with Hitachi, Ltd., where they succeeded in developing a basic technology of a high thermally durable all-solid-state lithium ion battery.

Prof. Eiji Saitoh and co-workers are developing thermoelectric device, in collaboration with NEC Corporation and NEC TOKIN Corporation, using a revolutionary quantum principle based on the "spin

Seebeck effect” which Saitoh group discovered. As of the end of FY2015, the device showed the conversion efficiency one million times higher than that in the early stage of development and has taken an important step towards practical use as a generator element.

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 2-4, list and describe media coverage, press releases, and reporting.

As shown in detail in **Appendix 2-4**, 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 colleges, 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. 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, 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. In FY2015, Specially-appointed Associate Professor Osamu Shimizu took over the outreach manager and he renewed the **AIMR MAGAZINE**.

The PR & Outreach Office asked AIMR laboratories to increase press releases by promising support for manuscripts, and tentatively initiated overseas-targeted press releases. As a result, many research results have appeared in the media, mainly in newspapers as shown in **Appendix 2-4**.

3. Interdisciplinary Research Activities (within 3 pages)

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

AIMR was established in FY2007 and four groups, Bulk Metallic Glasses (current Non-equilibrium Materials group), Material Physics, Soft Materials, and Device/System, were organized. It was difficult for these groups to intermingle with each other initially. In FY2009, AIMR started the “**Fusion Research Proposal Program**” to help researchers promote interdisciplinary fusion research between/among different research groups. So far, 135 proposals have been accepted (13, 14, 17, 10, 18, 22, 21, and 20) proposals in FY2009 (first half), FY2009 (latter half), FY2010, FY2011, FY2012, FY2013, FY2014, and FY2015, respectively, and funds were provided for the launch of new fusion research between/among different research groups. After the launch of this Fusion Research Proposal Program, 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 proceeded. 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 (Prof. Motoko Kotani; mathematician) and new Administrative Director (Prof. Masaru Tsukada; theoretical physicist), AIMR achieved great progress in **mathematics–materials science collaboration** which started at the end of FY2010, and its basis was almost completed in FY2011. The **Mathematics Unit** consisting of pure and applied mathematicians was established in March 2011, and two PIs (Prof. Yasumasa Nishiura, the leader of the unit, and Prof. Motoko Kotani) led this new unit. 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. Several independent young theoretical physicists and chemists with a mathematical background and also knowledge of materials science were selected through international recruitment. Interface Unit researchers have played the role of interpreters and bridged the gap between the mathematicians and materials scientists as well as conducting their own research. Through the efforts of Interface Unit researchers, it became possible that mathematicians and materials scientists directly talk to each other. In order to deepen AIMR’s mathematics-materials collaborations further, the Mathematics Unit and Interface Unit were integrated into the “**Mathematical Science Group**” on April 1st, 2015, and their research activity has proceeded to the next stage of collaboration.

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. 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. 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.

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 sometimes held.

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. Based on these efforts, AIMR has started the publication of **“SpringerBriefs in the Mathematics of Materials,”** the world’s first textbook (monograph) series for math-mate collaboration, and the introductory volume “Volume 1: A New Direction in Mathematics for Materials Science” was published in December 2015. The second and following volumes focusing on specific topics are under preparation for published.

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 1-8. 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) Medium-range order in glass structures by persistent homology (**Nanotechnology**)
- 8) Mathematical model for periodic structures observed along grain boundaries (**Materials Transactions**)
- 9) Nanoscale mechanical heterogeneity in a metallic glass (**Physical Review Letters**)
- 10) The atomic structure of nanoporous gold surface causing catalysis (**Nature Materials**)
- 11) Nanoporous gold reductive catalysts (**Journal of the American Chemical Society**)
- 12) Metallic glass Pd-catalyst with skeleton nanopores (**Chemical Communications**)
- 13) Bilayer graphene C₆Ca (**Proceedings of the National Academy of Sciences USA**)
- 14) Reduced graphene oxide for phototransistors (**ACS Nano**)
- 15) Electrically induced ferromagnetism in cobalt-doped titanium dioxide (**Science**)
- 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 4-1, 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.

[Non-equilibrium Materials Group (Bulk Metallic Glasses (BMG) Group before FY2015)]

Prof. A. Lindsay Greer: Head of the School of Physical Sciences (Former head of the Department of Materials Science and Metallurgy), University of Cambridge. He has carried out long-standing collaboration with Prof. D.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.

The late **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. Unfortunately, he died in 2015. During his lifetime, as well as placing Dr. Konstantinos Georgarakis (assistant professor) at AIMR, he himself stayed at AIMR 1-3 months every year, and carried out joint research with M.W. Chen's (PI, AIMR) and D.V. Louzguine's (PI, AIMR) groups on bulk metallic glasses.

[Materials Physics Group]

Prof. Alexander Shluger: Professor of University College London. He has his laboratory at AIMR and placed Dr. Filippo Federici Canova (postdoc) before FY2015 and is placing Dr. Moloud Kaviani (postdoc) after that. Prof. Shluger stays at AIMR several weeks every year and is carrying out joint research with the K. Akagi (Associate Professor, AIMR) group, the K. Kurihara (PI, AIMR) group and the D.V. 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 has carried out joint research with the T. Hitosugi (Junior PI, 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 placed Dr. Ling Zhang (assistant professor) at AIMR, and performed joint research to develop sensors by a combination of nanoporous metals which the M.W. 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 carried out joint research with the K. Nakajima (Junior PI, AIMR) group on polymers and soft materials. He sometimes placed young researchers, including Ph.D. students of his laboratory at the University of Massachusetts, at AIMR as visiting scientists for the collaboration.

Prof. Li-Jun Wan: The 9th President of University of Science and Technology of China. 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) was placed at Wan Laboratory at AIMR, and carried out joint research on molecular nanotechnology.

Prof. Kosmas Prassides, Former Professor of Durham University and an authority of molecular superconductors, joined AIMR. He was appointed to a full-time PI of AIMR in FY2014. He has already established his laboratory by employing some researchers and started their research.

[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. M. Esashi (PI, AIMR) based on their long collaboration. Until now, Dr. Yu-Ching Lin (associate professor), Dr. Yao-Chuang Tsai (postdoc), and Dr. Jörg Frömel (associate professor) have been 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. (Unfortunately, Prof. Gessner passed away in May 2016.)

Junior PIs: AIMR also assigned three talented world-leading young researchers, **Prof. Ali Khademhosseini** (associate professor of Harvard Medical School; became a full professor of Harvard

Medical School, as well as PI of AIMR, in FY2014), **Prof. Winfried Teizer** (associate professor of Texas A&M University; resigned a position as Junior PI of AIMR at the end of FY2014), and **Prof. Hongkai Wu** (associate professor of Hong Kong University of Science and Technology), to be “Junior PIs” in FY2009. They have a laboratory at AIMR, and employ three or four assistant professors and postdoctoral researchers. These 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.

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 4-2~4, 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 at least 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.

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 4-5, 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. In recent years, AIMR strengthened the relationship with the University of Chicago; AIMR and the University of Chicago signed the agreement in FY2014 and established a joint laboratory in FY2015. Postdoctoral researchers at AIMR have been employed and placed at the joint laboratories as shown below (Dr. Kiss and Dr. Zheng have left). 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 |
| Chicago | | |
| Prof. David Awschalom (Spintronics) | Dr. Gary Wolfowicz | Prof. Hideo Ohno |
| Prof. Paul Nealey (Chemistry) | Dr. Takuya Yanagimachi | Prof. Kazue Kurihara |

4-2. Center's Record of Holding International Symposia, Workshops, Research Meetings, Training Meetings and Others

- In Appendix 4-6, 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 1,800 attendees from over 15 countries (in total of 8 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 research 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. About ten researchers have utilized this dispatch program every year.

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.

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 International Advisory Board (holds yearly meetings) and the External Advisory Board 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 can provide services in English, was first established, and all office documents were translated into English. 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 concluding 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. The expertise has been inherited by the research reception center (International Affairs Center) which was 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 5-1, 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 5-2, 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 5-3, give the transition in the number of female researchers.

During the past nine 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 about twenty young mathematicians and theoretical researchers. 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% (7% for PI and 9% 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 has established "Graduate Program in Spintronics (GP-Spin)," where AIMR researchers are playing a central role and world-leading researchers and graduate students are gathering.

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 established a new system to invite administrative staff from overseas institutions; such invitations provide learning opportunities not only for dispatched staff, but also for all administrative members. So far, we received administrative staff from the Carnegie Institution for Science and University of Copenhagen.

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 FY2015 Follow-up (including Site Visit Results)

* Describe the Center's Response to Results of FY2015 Follow-up. Note: If you have already provided this information, please indicate where in the report.

[Suggestion 1]

AIMR is expected to create "new materials science capable of predicting new functions based on a mathematics-materials concept." This is a really challenging and long-term target, with the full-fledged fusion of materials science and mathematics remaining a challenge for the future. In addition, benefits for materials science are evident but not visible to mathematics. A two-way cognitive effort, i.e. mathematician learning from materials science and vice versa, is desired to achieve the center's ultimate objectives.

[Response]

The mathematics-materials science collaboration provides benefit not only to materials science but also mathematics and mathematicians. There is reciprocal benefit here. At AIMR, when mathematicians make mathematical models they can ask experimentalists to test the models and mathematicians can improve the models using the experimental results. Such place in which mathematicians can easily access the materials experimental environment is unprecedented. "SpringerBriefs in the Mathematics of Materials" (Editor-in-Chief M. Kotani), the monograph series whose publication was started in December 2015, are useful also materials scientists. However, this publication was proposed by an editorial staff of mathematics and the main target of the series is mathematicians. This is the clear evidence that the AIMR's mathematics-materials science collaboration give benefit to mathematics. Center Director Prof. Kotani has been invited to many universities, institutes and international conferences, for example, Institut Mittag-Leffler (Sweden), Centre International de Rencontres Mathématiques (France), the Australian National University (Australia), Institute for Mathematics and its Applications (IMA; at University of Minnesota, U.S.A.) and International Conference Computational and mathematical methods in Science and Engineering (CMMSE), to give a talk on the AIMR's mathematics-materials science collaboration and attracted much interest of the mathematical community.

[Suggestion 2]

OAS is highly evaluated for establishing its International Administrative Office and Graduate School of Spintronics, although it is not clear at present how they will be implemented. Continued efforts on institutional reform would be desirable.

[Response]

The administrative division of AIMR has already started the administrative works in OAS. International relation unit of the AIMR's administrative office has formed International Affairs Center (IAC) in OAS,

which is practically playing a role as a reception center of researchers from overseas. With respect to the Graduate School of Spintronics, the framework of "Graduate Program in Spintronics (GP-Spin)" has been completed by the strong support of Tohoku University and the leadership of Prof. Yoshiro Hirayama, the Project Coordinator of GP-Spin and an AIMR's Affiliated Professor. Based on the teaching and guidance by the world-leading faculty members, it is expected that the excellent students will grow into major researchers leading the future spintronics of the world.

World Premier International Research Center Initiative (WPI)

Appendix 1-1. FY 2015 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 Appendix1-1a, "Biographical Sketch of a New Principal Investigator".

| <Results at the end of FY2015> | | | | | | | | | |
|--|--|---|--|---------------------|------------------------|---------------------|--|---|---|
| Principal Investigators Total: 29 | | | | | | | | | |
| Name (Age) | Affiliation (Position title, department, organization) | Academic degree, specialty | Working hours (Total working hours: 100%) | | | | Starting date of project participation | Status of project participation (Describe in concrete terms) | Contributions by PIs from overseas research institutions |
| | | | Work on center project | | Others | | | | |
| | | | Research activities | Other activities | Research activities | Other activities | | | |
| Center director Motoko Kotani* (56) | 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* (58) | 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* (50) | Professor, AIMR, Tohoku University | Dr. of Engineering, Materials Science | 100% | 0% | 0% | 0% | From start | Usually stays at the center | |
| Masayoshi Esashi* (67) | Professor, AIMR, Tohoku University | Dr. of Engineering Sensors, Micro Electro Mechanical | 80% | 0% | 0% | 20% | From start | Usually stays at the center | |

| | | | | | | | | | |
|---------------------------|---------------------------------------|---|------|----|-----|-----|---|-----------------------------|--|
| | | Systems | | | | | | | |
| Hiroyuki Isobe* (45) | Professor, AIMR, Tohoku University | Ph.D., Organic Chemistry | 80% | 0% | 10% | 10% | From Apr. 2013 | Usually stays at the center | |
| Kazue Kurihara* (65) | Professor, AIMR, Tohoku University | Dr. of Engineering, Physical Chemistry, Colloid and Interface Science | 80% | 0% | 0% | 20% | From Apr. 2010 | Usually stays at the center | |
| Dmitri V. Louzguine* (48) | 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* (62) | Professor, AIMR, Tohoku University | Dr. of Pharmacy, Biosensing Engineering | 80% | 0% | 0% | 20% | From Nov. 2010 | Usually stays at the center | |
| Shigemi Mizukami* (43) | Professor, AIMR, Tohoku University | Dr. of Engineering, Applied Physics, Spintronics | 100% | 0% | 0% | 0% | From Nov., 2014 | Usually stays at the center | |
| Yasumasa Nishiura* (65) | Professor, AIMR, Tohoku University | Dr. of Science, Applied Mathematics (Nonlinear Dynamics) | 100% | 0% | 0% | 0% | From Feb. 2012 | Usually stays at the center | |

| | | | | | | | | |
|-------------------------|---|---|------|----|-----|-----|-------------------|---|
| Shin-ichi Orimo* (50) | Professor, AIMR, Tohoku University | Ph.D., Materials Engineering and Chemistry | 80% | 0% | 0% | 20% | From Jan. 2013 | Usually stays at the center |
| Kosmas Prassides* (58) | Professor, AIMR, Tohoku University | D.Phil. in Chemistry | 100% | 0% | 0% | 0% | From Apr. 2013 | Usually stays at the center |
| Eiji Saitoh* (44) | Professor, AIMR, Tohoku University | Dr. of Engineering, Spintronics | 80% | 0% | 0% | 20% | From Apr. 2012 | Usually stays at the center |
| Takashi Takahashi* (64) | Professor, AIMR, Tohoku University | Dr. of Science, Solid-State Physics | 80% | 0% | 0% | 20% | From start | Usually stays at the center |
| Katsumi Tanigaki* (61) | Professor, AIMR, Tohoku University | Dr. of Engineering, Nano Materials Science | 80% | 0% | 0% | 20% | From start | Usually stays at the center |
| Hideo Ohno* (61) | 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* (57) | Professor, Institute of Fluid Science, Tohoku University | Dr. of Engineering, Nanoprocess | 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* (57) | 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 |

| | | | | | | | | | |
|-----------------------------------|--|---|-----|----|-----|-----|----------------|--|---|
| <u>Tomasz Dietl</u> * (65) | Professor, Head of Laboratory of Cryogenic and Spintronic Research, Institute of Physics, Polish Academy of Sciences | Dr. Hab., physics of semiconductors and magnetic materials, low-temperature physics | 20% | 0% | 45% | 35% | From Apr. 2012 | <ul style="list-style-type: none"> • Stays at the center once (for two weeks) a year • Dispatches a researcher who belongs to the same institute with PI to give an invited lecture at the AIMR conference | |
| <u>Thomas Gessner</u> * (61) | Professor, Center for Microtechnologies, Chemnitz University of Technology | Ph.D. in Device Science/Technology | 30% | 0% | 50% | 20% | From start | <ul style="list-style-type: none"> • Stays at the center twice a year • Attends the AIMR conference • Sends young scientists to the center • Dispatches a researcher who belongs to the same institute with PI to give an invited lecture at the AIMR conference | Send young scientists to the WPI center (1/6.5 years since 2008) (1/2.3 years since 2012) (1/1 year) (1/6 months) |
| <u>Alain Lindsay Greer</u> * (60) | Professor, Department of Materials Science & Metallurgy, University of Cambridge | Ph.D. in Metallurgy & Materials Science | 20% | 0% | 45% | 35% | From start | <ul style="list-style-type: none"> • Stays at the center twice a year • Attends the AIMR conference • Sends young scientists to the center | Send young scientist to the WPI center (3/2 weeks each) (2/1 week each) |
| <u>Thomas P. Russell</u> * (63) | Professor, Department of Polymer Science and Technology, University of Massachusetts Amherst | Ph.D. in Nano-Science Technology | 20% | 0% | 45% | 35% | From start | <ul style="list-style-type: none"> • Stays at the center twice a year • Attends the AIMR conference | |
| <u>Alexander Shluger</u> * (61) | Professor, Department of Physics and Astronomy, University College London | Ph.D. in Computational Materials Science, Condensed Matter Physics | 35% | 0% | 45% | 25% | From start | <ul style="list-style-type: none"> • Stays at the center three times (one month in total) a year • Sends young scientists to the center • Dispatches a researcher who belongs to the same institute with PI to give an invited lecture at the AIMR conference | Send young scientists to the WPI center (1/2.4 years since 2012) (1/3 weeks) |

| | | | | | | | | | |
|----------------------------------|--|---|-----|----|-----|-----|-------------------|--|---|
| <u>Li-Jun Wan</u> * (58) | Professor, Institute of Chemistry, Chinese Academy of Science President of University of Science and Technology of China | Ph.D. in SPM, Physical Chemistry, Nanoscience and technology | 20% | 0% | 45% | 35% | From start | <ul style="list-style-type: none"> • Stays at the center once a year • Sends young scientists to the center | Send young scientist to the WPI center (1/1.5 years since 2013) |
| <u>Paul S. Weiss</u> * (56) | Professor, Department of Chemistry and Biochemistry, University of California, Los Angeles | Ph.D. in Surface Science | 20% | 0% | 45% | 35% | From start | <ul style="list-style-type: none"> • Sends young scientists to the center | Send young scientist to the WPI center (1/2.9 years since 2012) |
| <u>Qi-kun Xue</u> * (52) | Professor, Department of Physics, Tsinghua University | Ph.D. in Surface Science | 20% | 0% | 45% | 35% | From start | | |
| <u>Alain Reza Yavari</u> * (66) | Professor, Grenoble Institute of Technology | Ph.D. in Physical Metallurgy | 30% | 0% | 45% | 25% | From start | <ul style="list-style-type: none"> • Stays at the center twice (one month in total) a year • Attends the AIMR conference • Sends young scientists to the center | Send young scientists to the WPI center (1/6.9 years since 2008) (1/2 months) |
| <u>Ali Khademhosseini</u> * (40) | Professor, Medical School, Harvard University | Ph.D. in Bioengineeri ng | 35% | 0% | 45% | 20% | From Nov. 2009 | <ul style="list-style-type: none"> • Stays at the center twice a year • Joins a videoconference regularly from the home institution (Harvard Univ.) | Send young scientists to the WPI center (1/4.9 years since 2010) (1/4 years since 2011) (1/2.1 years since 2012) (1/1.5 months Since 2013) (1/7 months) |

| | | | | | | | | | |
|------------------------------|--|---------------------|-----|----|-----|-----|-------------------|--|--|
| <u>Winfried Teizer*</u> (45) | Associate Professor, Department of Physics, Texas A&M University | Ph.D. in Physics | 35% | 0% | 40% | 25% | From Nov. 2009 | <ul style="list-style-type: none"> • Stays at the center several times (more than four months in total) a year • Joins a videoconference regularly from the home institution (Texas A&M Univ.) | Send young scientists to the WPI center (1/4.4 years since 2010) (1/4.3 years since 2011) (1/3 months) |
|------------------------------|--|---------------------|-----|----|-----|-----|-------------------|--|--|

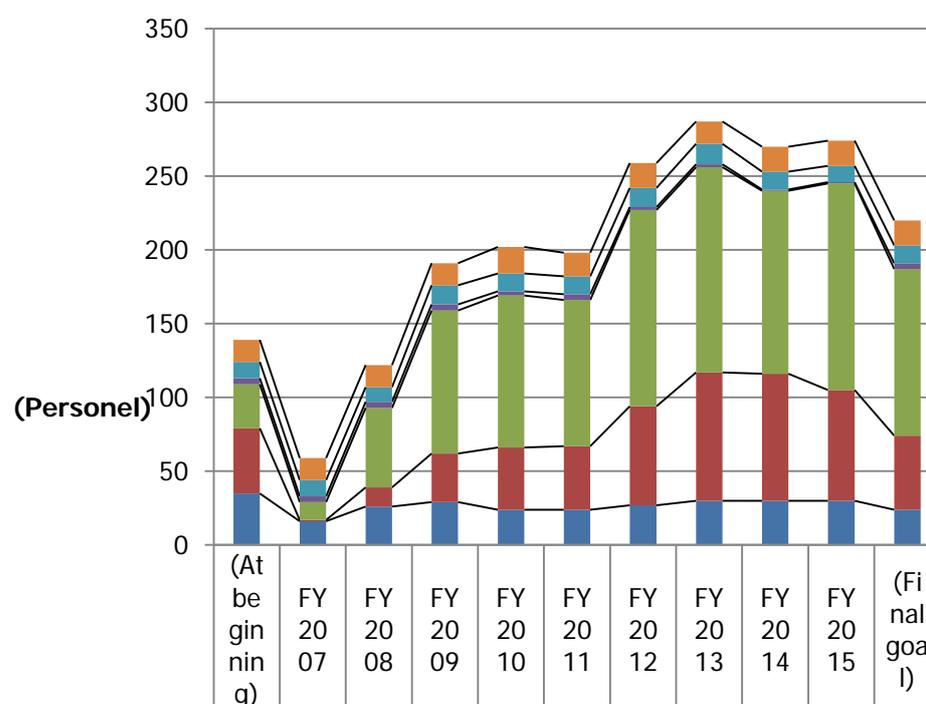
Researchers unable to participate in project in FY 2015

| Name | Affiliation (Position title, department, organization) | Starting date of project participation | Reasons | Measures taken |
|--------------------|--|--|---|----------------|
| <u>Hongkai Wu*</u> | Associate Professor, Department of Chemistry, Hong Kong University of Science and Technology | From Nov. 2009 | To concentrate on the research at the Department of Hong Kong University | |

World Premier International Research Center Initiative (WPI) Appendix 1-2. Annual Transition in the Number of Center Personnel

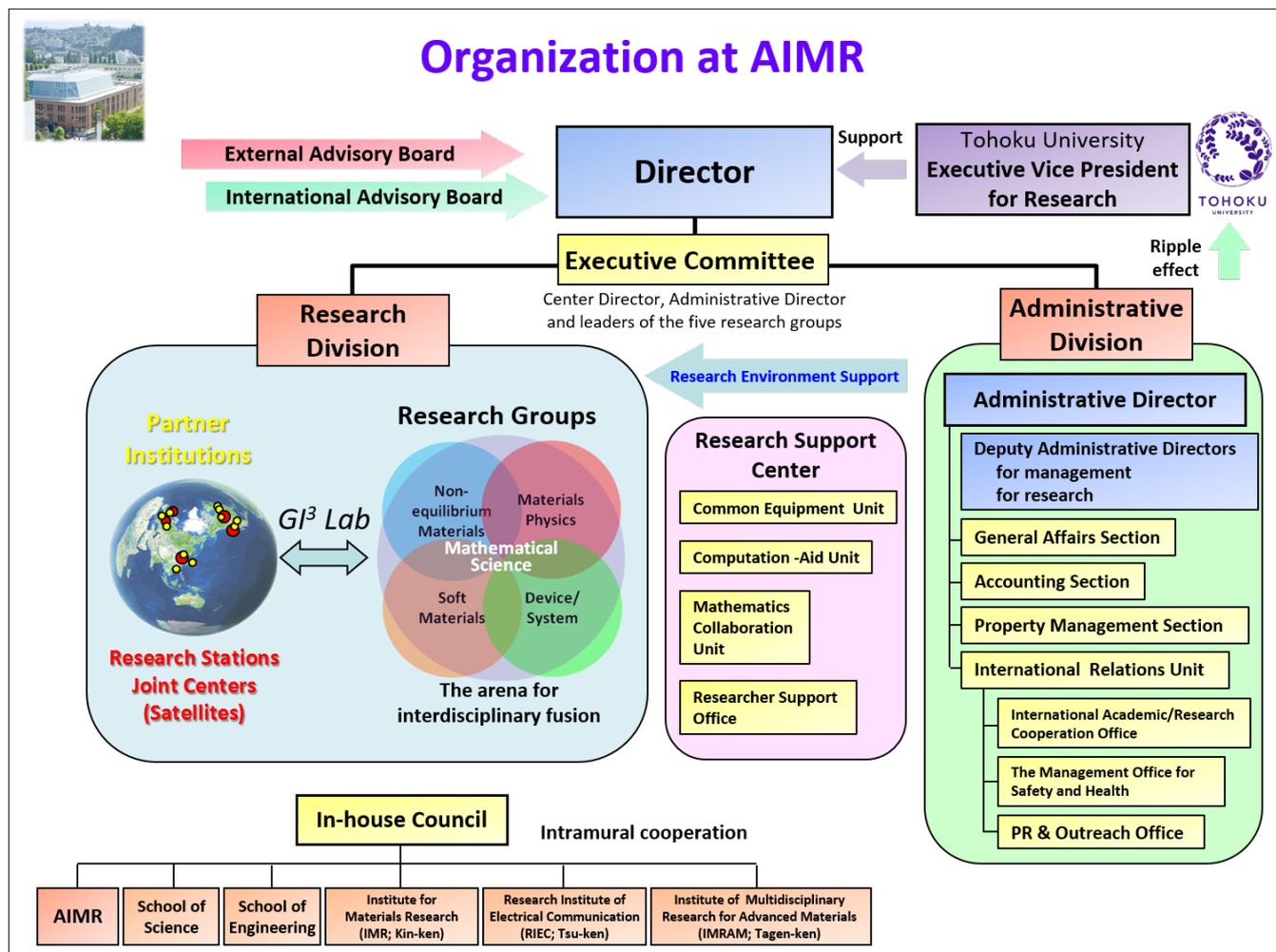
*Make a graph of the annual transition in the number of center personnel since the start of project.

Number of Center Personnel



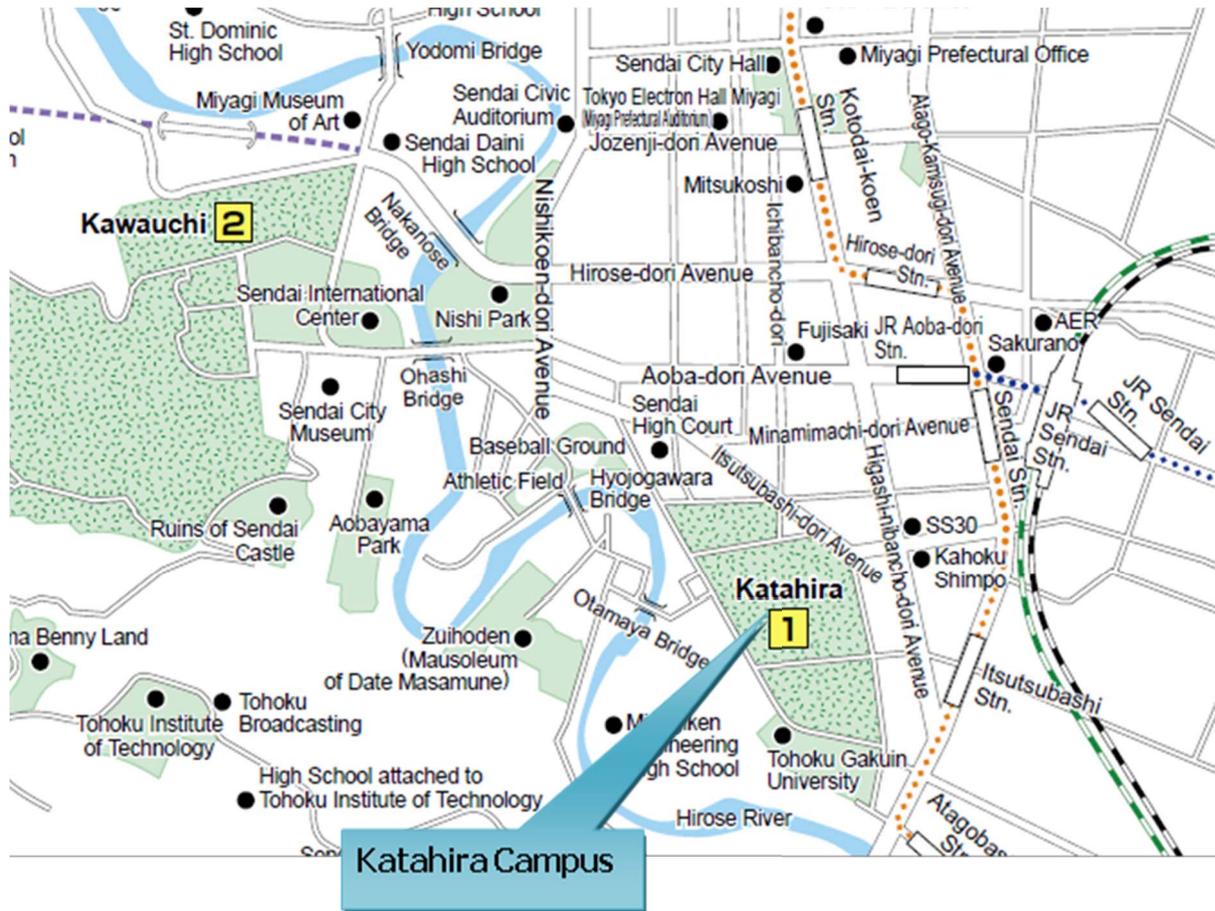
| | | | | | | | | | | | |
|---|----|----|----|----|-----|----|-----|-----|-----|-----|-----|
| PI : Researchers from within host institution | 15 | 15 | 15 | 15 | 18 | 16 | 17 | 15 | 17 | 17 | 17 |
| PI : Foreign researchers invited from abroad | 11 | 11 | 10 | 13 | 12 | 12 | 13 | 14 | 12 | 11 | 12 |
| PI : Researchers invited from other Japanese institutions | 4 | 4 | 4 | 4 | 3 | 4 | 2 | 2 | 1 | 1 | 4 |
| Other researchers | 30 | 12 | 54 | 97 | 103 | 99 | 133 | 139 | 124 | 140 | 113 |
| Research support staffs | 44 | 1 | 13 | 33 | 42 | 43 | 67 | 87 | 86 | 75 | 50 |
| Administrative staffs | 35 | 16 | 26 | 29 | 24 | 24 | 27 | 30 | 30 | 30 | 24 |

World Premier International Research Center Initiative (WPI) Appendix 1-3. Diagram of Management System

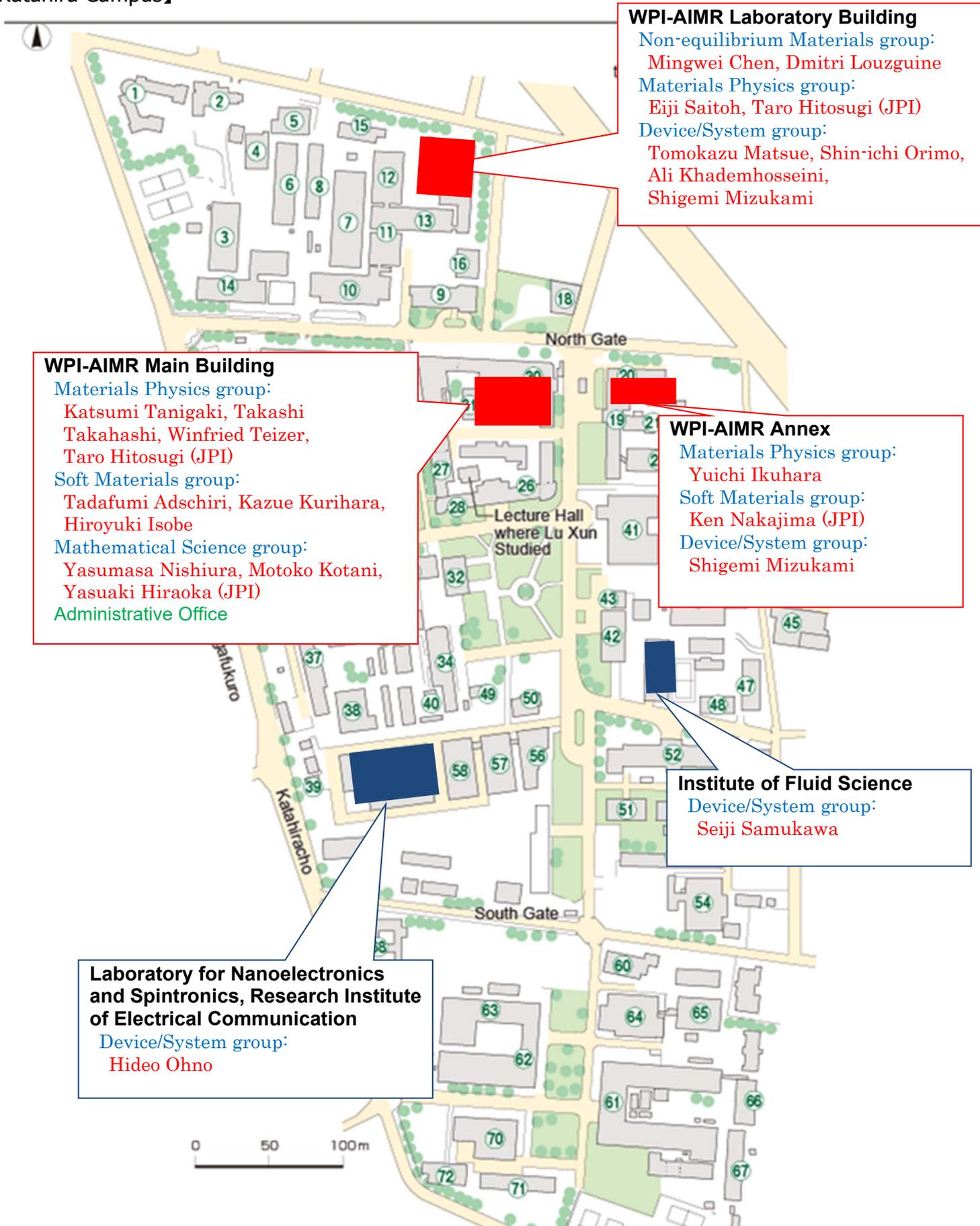


World Premier International Research Center Initiative (WPI) Appendix 1-4. Campus Map

4. Campus map



【Katahira Campus】

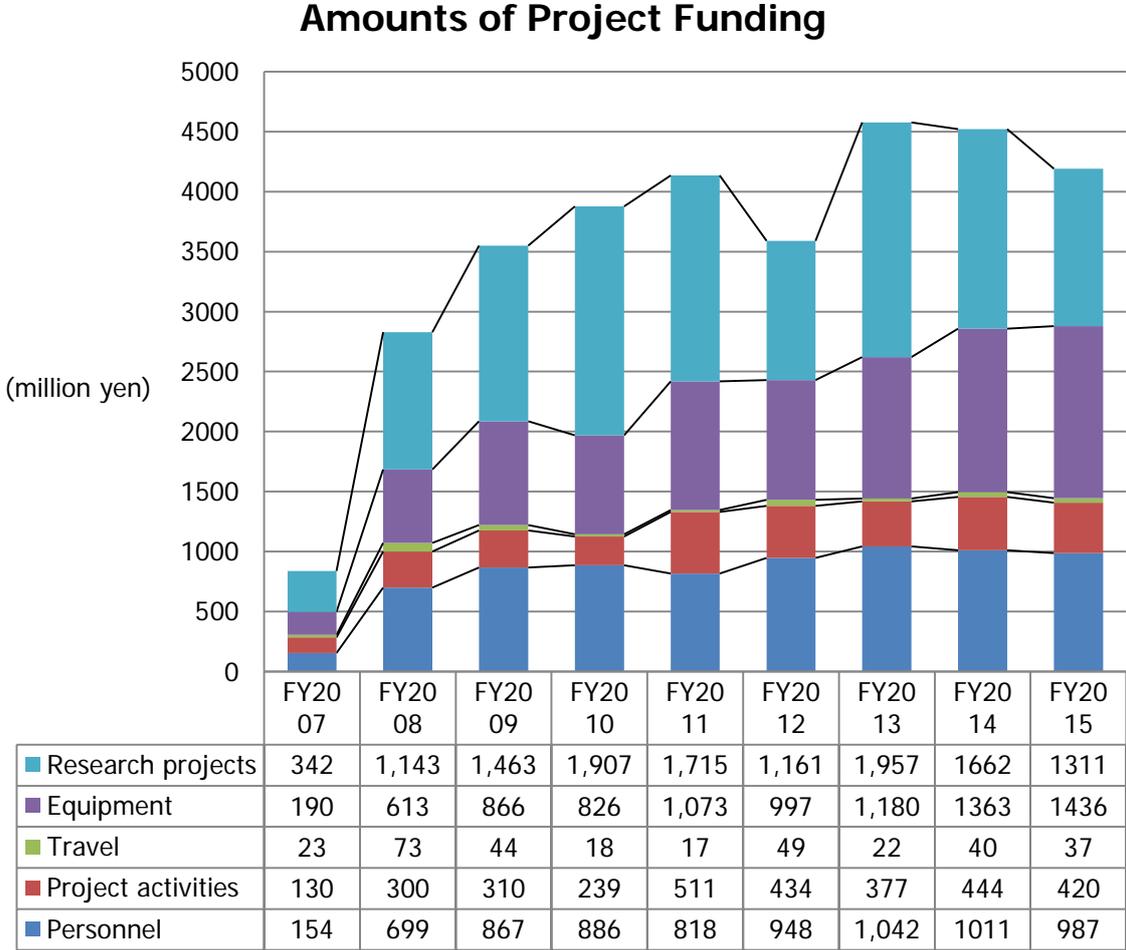


【Aobayama Campus】



World Premier International Research Center Initiative (WPI) Appendix 1-5. Annual Transition in the Amounts of Project Funding

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



Appendix 1-6. FY2015 Project Expenditures (the exchange rate used: 1USD= 100 JPY)

i) Overall Project Funding

| Cost Items | Details | Costs (10,000 dollars) | | Ten thousand dollars |
|----------------------------|--|---------------------------|--|----------------------|
| | | | WPI grant | 1285 |
| Personnel | Center director and Administrative director | 24 | | |
| | Principal investigators (no. of persons):17 | 194 | Cost of equipment procured | 990 |
| | Other researchers (no. of persons):95 | 539 | High Resolution, Horizontal X-ray Diffraction System | 40 |
| | Research support staffs (no. of persons):23 | 41 | Number of units: 1 Costs paid: | |
| | Administrative staffs (no. of persons):51 | 189 | Powder X-ray Diffraction System | 32 |
| | Total | 987 | Number of units: 1 Costs paid: | |
| Project activities | Gratuities and honoraria paid to invited principal investigators (no. of persons):12 | 13 | Inkjet Printing Test Equipment | 20 |
| | Cost of dispatching scientists (no. of persons): | | Number of units: 1 Costs paid: | |
| | Research startup cost (no. of persons):33 | 119 | Multipurpose High-Power X-Ray Diffraction System with Two-Dimensional Detector | 20 |
| | Cost of satellite organizations (no. of satellite organizations) | 27 | Number of units: 1 Costs paid: | |
| | Cost of international symposiums (no. of symposiums):1 | 37 | Nanomechanical Atomic Force Microscope | 15 |
| | Rental fees for facilities | | Number of units: 1 Costs paid: | |
| | Cost of consumables | 51 | Short-Pulse Oscillator for Amplifier Seeding | 13 |
| | Cost of utilities | 67 | Number of units: 1 Costs paid: | |
| | Other costs | 106 | The revolutionary platform for all-in-one characterization of solar cells and OLEDs | 13 |
| | Total | 420 | Number of units: 1 Costs paid: | |
| Travel | Domestic travel costs | 4 | Upgrade for Magnetron Sputtering System | 13 |
| | Overseas travel costs | 20 | Number of units: 1 Costs paid: | |
| | Travel and accommodations cost for invited scientists (no. of domestic scientists):5 (no. of overseas scientists):14 | 9 | Load-Lock Chamber | 13 |
| | Travel cost for scientists on secondment (no. of domestic scientists):6 (no. of overseas scientists):4 | 4 | Number of units: 1 Costs paid: | |
| | Total | 37 | Microminiature Gas Atomizing Apparatus | 12 |
| Equipment | Depreciation of buildings | 110 | Number of units: 1 Costs paid: | |
| | Depreciation of equipment | 1326 | Others | 799 |
| | Total | 1436 | | |
| Other research projects | Projects supported by other government subsidies, etc. | | | |
| | Commissioned research projects, etc. | 988 | | |
| | Grants-in-Aid for Scientific Research, etc. | 323 | | |
| | Total | 1311 | | |
| Total | | 4191 | | |

ii) Costs of Satellites and Partner Institutions

| Cost Items | Details | Costs (10,000 dollars) |
|----------------------------|--|---------------------------|
| Personnel | Principal investigators (no. of persons):1 | / |
| | Other researchers (no. of persons):10 | |
| | Research support staffs (no. of persons): | |
| | Administrative staffs (no. of persons): | |
| | Total | 56 |
| Project activities | | 40 |
| Travel | | 9 |
| Equipment | | |
| Other research projects | | |
| Total | | 105 |

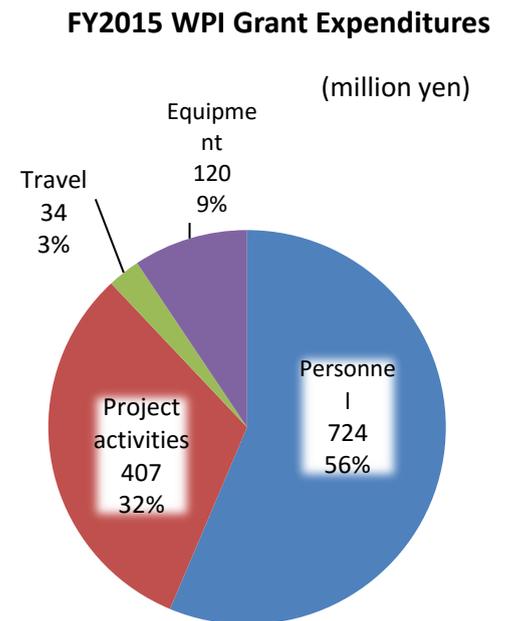
World Premier International Research Center Initiative (WPI)

Appendix 1-7. FY2015 WPI Grant Expenditures (the exchange rate used: 1USD= 100 JPY)

i) Overall Expenditures

* Describe a circle graph for cost items.

| Cost Items | Details | Costs (10,000 dollars) |
|--------------------|--|---------------------------|
| Personnel | Center director and Administrative director | 11 |
| | Principal investigators (no. of person):17 | 60 |
| | Other researchers (no. of person):95 | 501 |
| | Research support staffs (no. of person):14 | 30 |
| | Administrative staffs (no. of person):41 | 122 |
| | Total | 724 |
| Project activities | Gratuities and honoraria paid to invited principal investigators (no. of person):12 | 13 |
| | Cost of dispatching scientists (no. of person) | |
| | Research startup cost (no. of person):33 | 129 |
| | Cost of satellite organizations (no. of satellite organization):2 | 27 |
| | Cost of international symposiums (no. of symposiums):1 | 37 |
| | Rental fees for facilities | |
| | Cost of consumables | 44 |
| | Cost of utilities | 65 |
| | Other costs | 92 |
| | Total | 407 |
| Travel | Domestic travel costs | 3 |
| | Overseas travel costs | 18 |
| | Travel and accommodations cost for invited scientists (no. of domestic scientists):5 | 9 |
| | Travel cost for scientists on secondment (no. of domestic scientists):6 (no. of overseas scientists):4 | 4 |
| | Total | 34 |
| Equipment | Cost of equipment procured | 120 |
| | Total | 120 |
| Total | | 1285 |



ii) Costs of Satellites and Partner Institutions

| Cost Items | Details | Costs (10,000 dollars) |
|--------------------|---|---------------------------|
| Personnel | Principal investigators (no. of person):1 | / |
| | Other researchers (no. of person):10 | |
| | Research support staffs (no. of person) | |
| | Administrative staffs (no. of person) | |
| Total | | 56 |
| Project activities | | 40 |
| Travel | | 9 |
| Equipment | | |
| Total | | 105 |

World Premier International Research Center Initiative (WPI) Appendix 2-1. 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. K. Iwaya, T. Ogawa, T. Minato, K. Miyoshi, J. Takeuchi, A. Kuwabara, H. Moriwake, Y. Kim, T. Hitosugi, Impact of Lithium-Ion Ordering on Surface Electronic States of Li_xCoO₂. **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. Z.C. Wang, M. Okude, M. Saito, S. Tsukimoto, A. Ohtomo, M. Tsukada, M. Kawasaki and Y. Ikuhara, 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. Z.C. Wang, M. Saito, K.P. McKenna, L. Gu, S. Tsukimoto, A.L. Shluger and Y. Ikuhara, 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. Z.C. Wang, M. Saito, K. P. McKenna and Y. Ikuhara, 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.

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

- *6. K. Sugawara, T. Sato and T. Takahashi, 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 be 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. P. Richard, 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 T. Takahashi, Observation of Dirac cone electronic dispersion in $BaFe_2As_2$. **Physical Review Letters** 104, 137001 (2010).

Dirac cone in iron-based superconductors: 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, S. Souma, K. Nakayama, K. Eto, T. Minami, Y. Ando and T. Takahashi, 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. Y. Tanaka, Z. Ren, T. Sato, K. Nakayama, S. Souma, T. Takahashi, 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. D. Wang, S. Fujinami, K. Nakajima and T. Nishi, 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. T. Fujita, K. Konno, W. Zhang, V. Kumar, M. Matsuura, A. Inoue, T. Sakurai and M.W. Chen, 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. A. Hirata, P. Guan, T. Fujita, Y. Hirotsu, A. Inoue, A. R. Yavari, T. Sakurai and M.W. Chen, Direct observation of local atomic order in a metallic glass. **Nature Materials** 10, 28-33 (2011).

Discovery of a short-range order and clusters in BMG: 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. A. Hirata, T. Fujita, Y.R. Wen, J.H. Schneibel, C.T. Liu and M.W. Chen, Atomic structure of nanoclusters in oxide-dispersion-strengthened steels. **Nature Materials** 10, 922-926 (2011).

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. S. V. Ketov, Y. H. Sun, S. Nachum, Z. Lu, A. Checchi, A. R. Beraldin, H. Y. Bai, W. H. Wang, D. V. Louzguine-Luzgin, M. A. Carpenter and A. L. Greer, Rejuvenation of metallic glasses by non-affine thermal strain. **Nature** 524, 200–203 (2015).

Rejuvenation by thermal treatment: Metallic glasses have atomic arrangement closer to that of liquids than of conventional alloys which have crystalline structures. This structure imparts metallic glasses with high strength and toughness. However, metallic glasses generally become more brittle over time and increasingly susceptible to cracking. In this study, an AIMR's international team lead by Cambridge Satellite found an unexpectedly simple way to reverse this aging by simple thermal cycling between room temperature and liquid-nitrogen temperature (77 kelvin). If metallic glasses had truly featureless structures, such thermal cycling would have no effect. But, in reality, relatively gentle thermal cycling has very significant effects, equivalent to those of much more extreme processing. This result caused by thermal effect suggests that metallic glasses cannot be completely homogeneous, inhomogeneity in nanoscale probably exists in metallic glasses.

[Control atoms and molecules]

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

- *15. K. Ueno, S. Nakamura, H. Shimotani, A. Ohtomo, N. Kimura, T. Nojima, H. Aoki, Y. Iwasa and M.

Kawasaki, Electric-field-induced superconductivity in an insulator. **Nature Materials** 7, 855–858 (2008).

Manifestation of Superconductivity by Field-Effect Doping: Strontium titanate (SrTiO_3) 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 SrTiO_3 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. A. Tsukazaki, S. Akasaka, K. Nakahara, Y. Ohno, H. Ohno, D. Maryenko, A. Ohtomo and M. Kawasaki, Observation of the fractional quantum Hall effect in an oxide. **Nature Materials** 9, 889–893 (2010).

Fractional Quantum Hall Effect in an Oxide Material: 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.

- *17. 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).

Transparent superconductors by stoichiometry control: 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"

- *18 L. Chen, F. Matsukura, and H. Ohno, 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 measurable 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.

- *19. 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 E. Saitoh, "Unidirectional spin-wave heat conveyor" **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 $\text{Y}_3\text{Fe}_5\text{O}_{12}$. 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.

- *20. T. Arakane, T. Sato, S. Souma, K. Kosaka, K. Nakayama, M. Komatsu, T. Takahashi, Z. Ren, K. Segawa and Y. Ando, Tunable Dirac cone in the topological insulator $\text{Bi}_{2-x}\text{Sb}_x\text{Te}_{3-y}\text{Se}_y$. **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 Molecular superconductors

- *21. R.H. Zadik, Y. Takabayashi, G. Klupp, R.H. Colman, A.Y. Ganin, A. Potočník, P. Jeglič, D. Arčon, P. Matus, K. Kamarás, Y. Kasahara, Y. Iwasa, A.N. Fitch, Y. Ohishi, G. Garbarino, K. Kato, M.J. Rosseinsky and K. Prassides, Optimized unconventional superconductivity in a molecular Jahn–Teller metal. **Science Advances** 1, e1500059 (2015).

T_c dome and a molecular Jahn–Teller metal: Molecular superconductors are characterized by periodic

arrangements of molecules. Molecular superconductors that have an ordered lattice of fullerene molecules (C_{60}) and alkali-metal atoms currently boast the highest critical temperature (38 kelvin) of all known molecular superconductors. An international team led by AIMR researchers investigated one of such molecular superconductors, cesium fulleride (Cs_3C_{60}). By replacing some of its cesium atoms with smaller rubidium atoms the researchers could vary the distance between adjacent fullerene molecules within the periodic structure. This substitution of smaller atoms mimics the effect of increasing the hydrostatic pressure. They found that critical temperature has a dome-like variation with the density of fulleride molecules. They also identified a new metallic phase, which they termed “a Jahn-Teller metal” because delocalized, metallic electrons coexist with electrons localized on the fullerene molecules.

- *22. S. Heguri, N. Kawade, T. Fujisawa, A. Yamaguchi, A. Sumiyama, K. Tanigaki and M. Kobayashi, Superconductivity in the graphite intercalation compound BaC_6 . **Physical Review Letters** 114, 247201 (2015).

Superconductivity in intercalation compounds: BaC_6 belongs to a group of materials known as graphite intercalation compounds (GICs), which consist of two-dimensional graphite sheets with metal atoms sandwiched, or intercalated, between them. Many GICs are considered to be conventional superconductors. However, one important observation for this family had been missing for many years, that of BaC_6 . In this study, AIMR researchers and collaborators at the University of Hyogo observed the superconductivity in the compound BaC_6 for the first time. Historically, the superconducting mechanism of GIC superconductors has been understood in the framework of the conventional electron-pairing mechanism. However, their experimental results suggest that some other factors should be considered for a complete description. They anticipate that this finding will advance the understanding of two-dimensional superconductivity.

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

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

Observation of interface dynamics: 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 Molecular motors

- *24. A. Sikora, J. Ramoń-Azcoń, K. Kim, K. Reaves, H. Nakazawa, M. Umetsu, I. Kumagai, T. Adschiri, H.

Shiku, T. Matsue, W. Hwang and W. Teizer, Molecular motor-powered shuttles along multi-walled carbon nanotube tracks. **Nano Letters** 14, 876–881 (2014).

Molecular conveyor belt: Miniature chemical reactors are increasingly being used to analyze biological samples. Unfortunately, the bulky pumps and batteries needed to operate such devices limit their further miniaturization and prevent them from being directly implanted into the body for monitoring applications. In this study, AIMR researchers developed a much smaller system that uses a natural motor protein, Kinesin-1, to transport cargo along a track made of carbon nanotubes. They used multiwalled carbon nanotubes for the track, and arrange them on a substrate by utilizing dielectrophoresis process with applied voltage. They covered the nanotubes with kinesin bearing a biotin linker, and then added adenosine triphosphate (ATP) as energy. Consequently, the kinesin molecules glided along the track at an average speed of around 150 nanometers per second. It is expected this will be applied to transportation of viruses, drugs, proteins or nanoparticles in the body as well as biosensing.

- *25. H. Isobe, K. Nakamura, S. Hitosugi, S. Sato, H. Tokoyama, H. Yamakado, K. Ohno and H. Kono, Theoretical studies on a carbonaceous molecular bearing: association thermodynamics and dualmode rolling dynamics. **Chemical Science** 6, 2746-2753 (2015).

Molecular bearing: A team engaging in nanocarbon molecule synthesis at AIMR succeeded in synthesizing a carbonaceous molecular bearing comprising a belt-persistent tubular molecule and a fullerene molecule in 2013. In this study, the team investigated the rotational motion of the molecular bearing based on leading-edge theoretical calculations using density functional theory (DFT). Among ten representative methods, two DFT methods afforded an association energy that reasonably reproduced the experimental enthalpy of $-12.5 \text{ kcal mol}^{-1}$ at the unique curved π -interface. The dynamics of the molecular bearing, which was assembled solely with van der Waals interactions, exhibited small energy barriers with maximum values of 2–3 kcal mol^{-1} for the rolling motions. The dynamic motions responded sensitively to the steric environment and resulted in two distinct motions, precession and spin, which explained the unique NMR observations that were not clarified in previous experimental studies.

[Create new materials]

*Research results 11 Metallic glass nanowire

- *26. K.S. Nakayama, Y. Yokoyama, T. Ono, M.W. Chen, K. Akiyama, T. Sakurai and A. Inoue, Controlled formation and mechanical characterization of metallic glassy nanowires. **Advanced Materials** 22, 872–875 (2010).

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, T. Adschiri 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).

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. X. Lang, A. Hirata, T. Fujita and M.W. Chen, Nanoporous metal/oxide hybrid electrodes for electrochemical supercapacitors. **Nature Nanotechnology** 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 Three-dimensional nanoporous graphene

- *30. Y. Ito, Y. Tanabe, H.-J. Qiu, K. Sugawara, S. Heguri, Ngoc Han Tu, Khuong Kim Huynh, T. Fujita, T. Takahashi, K. Tanigaki, M.W. Chen, High-quality three-dimensional nanoporous graphene. **Angewandte Chemie International Edition** 53, 4822-4826 (2014).

Creation of highly crystalline three-dimensional nanoporous graphene: Turning graphene sheets into complex three-dimensional (3D) networks is a hard task. Template-assisted growth method developed recently can successfully produce 3D graphene, but the electron mobility is low due to discontinuous or rough surfaces that introduce defects into the 3D framework. The AIMR researchers developed an improved template with a structure containing a continuous, smooth surface of nickel atoms and continuous nanoscale pores. Uniform films of graphene all over the nickel template grew by chemical vapor deposition (CVD) method with hydrogen, argon and benzene gases, and finally, nickel was removed by acid. The obtained 3D nanoporous graphene shows high electron mobility because of high crystallinity and is applicable to a low-cost and ecofriendly alternative to gas sensors, transistors or energy-harvesting devices such as lithium–air batteries.

*Research results 15 Biomaterials

- *31. J. Ramón-Azcón, S. Ahadian, R. Obregón, G. Camci-Unal, S. Ostrovidov, V. Hosseini, H. Kaji, K. Ino, H. Shiku, A. Khademhosseini and T. Matsue, 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. T. Fujie, Y. Mori, S. Ito, M. Nishizawa, H. Bae, N. Nagai, H. Onami, T. Abe, A. Khademhosseini, and H Kaji, Micropatterned polymeric nanosheets for local delivery of an engineered epithelial monolayer. **Advanced Materials** 26, 1699-1705 (March 2014).

Ultrathin polymer-based “nanosheets”: 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, Y.M. Li and S. Samukawa, 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. T.J. Udovic, M. Matsuo, W.S. Tang, H. Wu, V. Stavila, A.V. Soloninin, R.V. Skoryunov, O.A. Babanova, A.V. Skripov, J.J. Rush, A. Unemoto, H. Takamura and S. Orimo, Exceptional superionic conductivity in disordered sodium decahydro-closo-decaborate. **Advanced Materials** 26, 7622–7626 (2014).

For all-solid-state rechargeable batteries: Solid electrolytes are superior for use in rechargeable batteries for safety reasons. Lithium-based solid electrolytes are currently the best performers. However, due to the relative scarcity of lithium, researchers are searching for alternative materials made from more abundant elements. In this study, along with overseas collaborators, AIMR researchers have discovered a potential rival to lithium-based electrolytes, a complex hydride containing the metals sodium and boron ($\text{Na}_2\text{B}_{10}\text{H}_{10}$). They found that the sodium-ion conductivity suddenly leapt by almost a hundredfold when the temperature reached about 110 degrees Celsius. The researchers consider that the “reorientational motion” of the anion columns $\text{B}_{10}\text{H}_{10}$ in the structure in some way assists the sodium ions as they travel through the corridors. In the future, by reducing the onset temperature to close to room temperature, construction of all-solid-state sodium rechargeable batteries is hoped using this material.

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

- *35. S. Mizukami, F. Wu, A. Sakuma, J. Walowski, D. Watanabe, T. Kubota, X. Zhang, H. Naganuma, M. Oogane, Y. Ando and T. Miyazaki, 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. X. Zhang, S. Mizukami, T. Kubota, Q. Ma, M. Oogane, H. Naganuma, Y. Ando, and T. Miyazaki, 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 (C₆₀) 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. D. Ishii, H. Yabu, and M. Shimomura, 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. Y. Takahashi, A. I. Shevchuk, P. Novak, B. Babakinejad, J. Macpherson, P. R. Unwin, H. Shiku, J. Gorelik, D. Klenerman, Y. E. Korchev and T. Matsue, 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, Y. Takahashi, H. Shiku, and T. Matsue, 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.

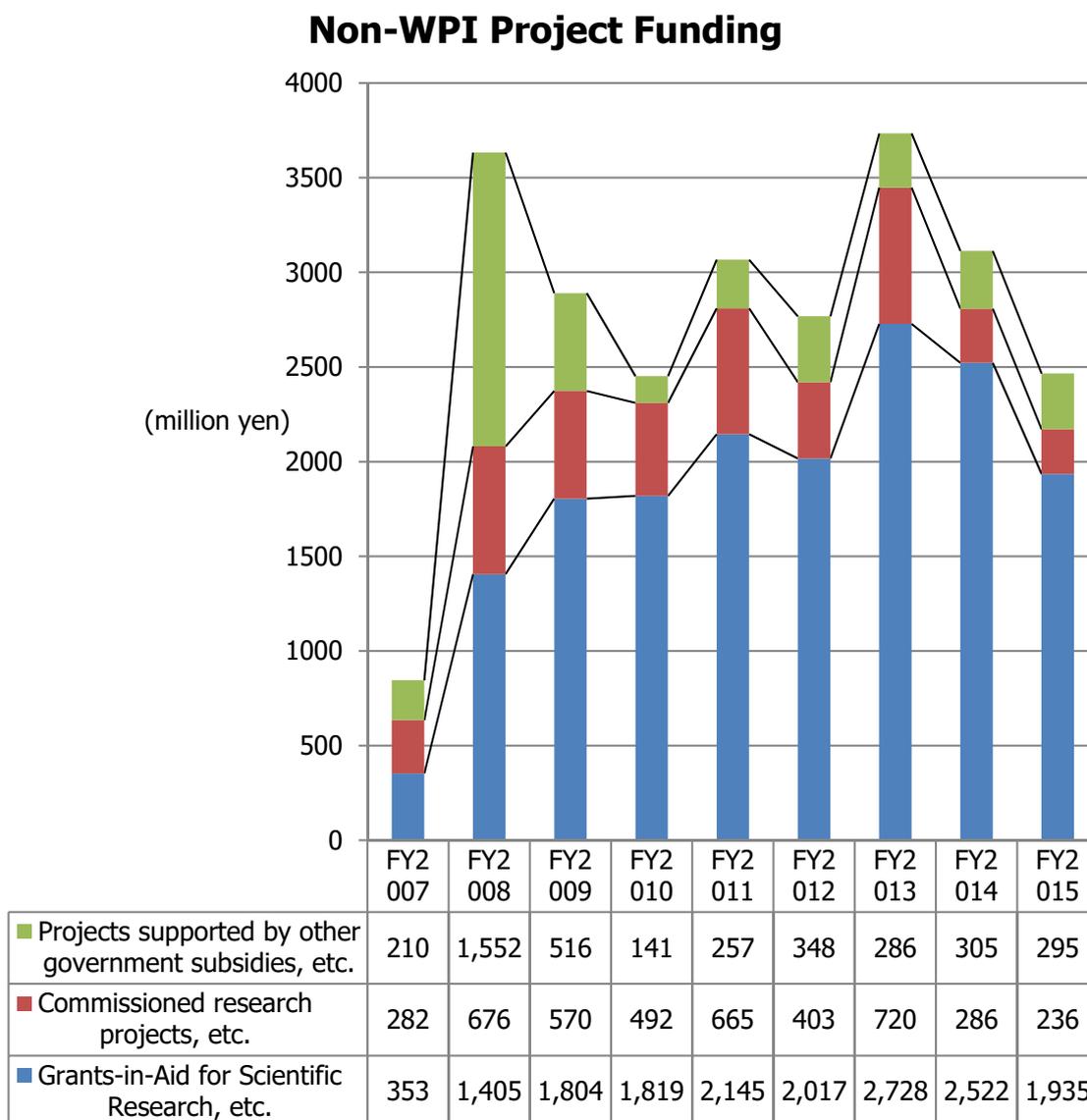
*Research results 20 Micro Electro Mechanical System (MEMS)

- *40. J.-W. Lee, Y.-C. Lin, N. Kaushik, P. Sharma, A. Makino, A. Inoue, M. Esashi and T. Gessner, Micromirror 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.

World Premier International Research Center Initiative (WPI) Appendix 2-2. 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) (FY2008-FY2013) : 1,557 million yen

Chief Researcher : Prof. Hideo Ohno

Total amount(JPY) (FY2008-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 (ERATO)】

Chief Researcher : Prof. Hiroyuki Isobe
 Total amount(JPY)(FY2013-) : 850 million yen
 Chief Researcher : Prof. Eiji Saitoh
 Total amount (FY2014-) : 433 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) : 238 million yen
 Chief Researcher : Prof. Motoko Kotani
 Total amount(JPY)(FY2011-FY2013) : 120 million yen
 Chief Researcher : Prof. Eiji Saito
 Total amount(JPY)(FY2012-FY2013) : 51 million yen

【Gran-in-Aid for Scientific Research Scientific Research S】

Chief Researcher : Prof. Masanobu 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. Takashi Takahashi
 Total amount(JPY)(FY2011-FY2013) : 180 million yen
 Chief Researcher : Prof. Masahiko Yamaguchi
 Total amount(JPY)(FY2009-FY2011) : 127 million yen
 Chief Researcher : Prof. Shin-ichi Orimo
 Total amount(JPY)(FY2013-) : 125 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

【Advanced Low Carbon Technology Research and Development Program (ALCA)】

Chief Researcher : Prof. Tomokazu Matsue
 Total amount (FY2013-) : 20 million yen
 Chief Researcher : Lectuer Atsushi Unemoto
 Total amount (FY2013-) : 29 million yen

【Development of Systems and technology】

Chief Researcher : Prof. Tomokazu Matsue
 Total amount (FY2012-) : 114 million yen

【Adaptable and Seamless Technology transfer Program (A-Step)】

Chief Researcher : Associate Prof. Koji Nakayama

Total amount (FY2013-) : 19 million yen

【Cross-ministerial Strategic Innovation Promotion Program (SIP)】

Chief Researcher : Prof. Kazue Kurihara

Total amount (FY2014-) : 50 million yen

Chief Researcher : Prof. Tadafumi Adschiri

Total amount (FY2014-) : 107 million yen

Chief Researcher : Prof. Yasumasa Nishiura

Total amount (FY2014-) : 37 million yen

【Advanced research program for energy and environmental technologies】

Chief Researcher : Prof. Tadafumi Adschiri

Total amount(FY2014- FY2015) : 54 million yen

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

1. Major Awards

*List main internationally-acclaimed awards received/unofficially 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.

- 1) **Yuichi Ikuhara**, 2015 Robert B. Sosman Award, the Basic Science Division, the American Ceramic Society, 2015.
- 2) **Shin-ichi Orimo**, Science of Hydrogen & Energy Award 2015.
- 3) **Masayoshi Esashi**, IEEE Andrew S. Grove Award 2015.
- 4) **Mingwei Chen**, Materials Today Conference Award, 2014.
- 5) **Mingwei Chen, Takashi Takahashi and Ali Khademhosseini**, named as Thomson Reuters Highly Cited Researchers 2014.
- 6) **Takashi Takahashi**, The 11th Honda Frontier Award, 2014.
- 7) **Kosmas Prassides**, Royal Society Wolfson Research Merit Award, February 2014.
- 8) **Ali Khademhosseini**, Elected AAAS(American Association for the Advancement of Science) Fellow, 2013.
- 9) **Alexander Shluger**, 2013 Daiwa Adrian Prizes, 2013.
- 10) **Taro Hitosugi**, Gottfried Wagener Prize 2013, 3rd prize, 2013.
- 11) **Kazue Kurihara**, Selected as the "IUPAC 2013 Distinguished Women in Chemistry or Chemical Engineering", 2013.
- 12) **Hideo Ohno**, Fellow of American Physical Society, 2012.
- 13) **Hideo Ohno**, IEEE David Sarnoff Award, 2012.
- 14) **Yuichi Ikuhara**, Fellow, The American Ceramic Society, 2011.
- 15) **Ali Khademhosseini**, Presidential Early Career Award for Scientists and Engineers (PECASE), 2011.
- 16) **Alain Reza Yavari**, Award for Scientific Excellence, French National Center for Scientific Research (CNRS), 2011.
- 17) **Kingo Itaya**, The Prix Jacques Tacussel Award of the International Society of Electrochemistry, 2011.
- 18) **Yuichi Ikuhara**, Humboldt Research Award, 2011.
- 19) **Kazue Kurihara**, A. E. Alexander Lecture Award 2011, The Royal Australian Chemical Institute, 2011.
- 20) **Yoshinori Yamamoto**, Centenary Prize 2009, Royal Society of Chemistry, UK, 2009.
- 21) **Toshio Nishi**, International Rubber Conference Organization (IRCO) Medal, 2009.
- 22) **Akihisa Inoue**, James C. McGroddy Prize for New Materials, American Physical Society, 2009.
- 23) **Terunobu Miyazaki**, Oliver E. Buckley Condensed Matter Prize, American Physical Society, 2009.
- 24) **Terunobu Miyazaki**, Asahi Prize, 2008.
- 25) **Yoshinori Yamamoto**, Arthur C. Cope Scholar Award, American Chemical Society, 2007.

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)

- 1) **Eiji Saitoh**, "Spin current generators," 20th International Conference on Magnetism (ICM 2015), Barcelona, Spain, July 8, 2015 (**Plenary Address**)
- 2) **Tomokazu Matsue**, "Electrochemical Imaging with Micro/Nanoelectrode Systems," The 66th International Society of Electrochemistry Annual Meeting, Taipei, Taiwan, October 5, 2015 (**Plenary Address**)

- 3) **Kosmas Prassides**, "Strongly correlated molecular superconductors," 11th International Conference on Materials & Mechanisms of Superconductivity (M2S HTSC 2015), Geneva, Switzerland, August 23-28, 2015 (**Plenary Address**)
- 4) **Shin-ichi Orimo**, "Cool hydrides, again!," 9th International Symposium "Hydrogen & Energy," Emmetten, Switzerland, January 25-30, 2015 (**Commemorative Lecture** for Science of Hydrogen & Energy Award 2015)
- 5) **Seiji Samukawa**, "Neutral Beam Technology - Defect-free Nanofabrication of Novel Nanomaterials," 14th IEEE International Conference on Nanotechnology, Toronto, Canada, August 21, 2014 (**Plenary Address**)
- 6) **Mingwei Chen**, "Ultrastable metallic glasses," International Symposium on Metastable, Amorphous and Nanostructured Materials (ISMANAM) 2014, Cancún, México, June 29 to July 4, 2014 (**Plenary Address**)
- 7) **Tadafumi Adschiri**, "Supercritical Route for Materials Synthesis," 14th European Meeting on Supercritical Fluids, Marseilles, France, May 21, 2014 (**Plenary Address**)
- 8) **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, Daejeon, Korea, March 21, 2014 (**Plenary Address**)
- 9) **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 Lecture**)
- 10) **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 Address**)
- 11) **Takashi Takahashi**, "Spin-resolved ARPES study of topological insulators and superconductors," 10th International conference on Spectroscopies in Novel Superconductors, Berkeley, U.S.A., June 24-28, 2013 (**Invited Talk**)
- 12) **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**)
- 13) **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
- 14) **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 Address**)
- 15) **Dmitry V. Louzguine**, "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**)
- 16) **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
- 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, August 16, 2009 (**Plenary Address**)

World Premier International Research Center Initiative (WPI)

Appendix 2-4. List of Achievements of Center's Outreach Activities

* Using the table below, show the achievements of the Center's outreach activities from FY2007 through FY2015 (number of activities, times held).

| Activities | FY2007 (number of activities, times held) | FY2008 (number of activities, times held) | FY2009 (number of activities, times held) |
|--|---|---|---|
| PR brochure, pamphlet | 0 | 0 | 1 |
| Lectures, seminars for general public | 38 | 30 | 33 |
| Teaching, experiments, training for elementary and secondary school students | 1 | 1 | 1 |
| Science cafe | 0 | 0 | 1 |
| Open houses | 1 | 1 | 1 |
| Participating, exhibiting in events | 3 | 3 | 3 |
| Press releases | 1 | 3 | 3 |

| Activities | FY2010 (number of activities, times held) | FY2011 (number of activities, times held) | FY2012 (number of activities, times held) |
|--|---|---|---|
| PR brochure, pamphlet | 3 | 13 | 5 |
| Lectures, seminars for general public | 28 | 22 | 4 |
| Teaching, experiments, training for elementary and secondary school students | 0 | 5 | 7 |
| Science cafe | 0 | 0 | 3 |
| Open houses | 1 | 5 | 2 |
| Participating, exhibiting in events | 3 | 13 | 6 |
| Press releases | 10 | 28 | 26 |

| Activities | FY2013 (number of activities, times held) | FY2014 (number of activities, times held) | FY2015 (number of activities, times held) |
|--|---|---|---|
| PR brochure, pamphlet | 7 | 19 | 4 |
| Lectures, seminars for general public | 7 | 30 | 27 |
| Teaching, experiments, training for elementary and secondary school students | 17 | 11 | 9 |
| Science cafe | 3 | 3 | 3 |
| Open houses | 2 | 1 | 1 |
| Participating, exhibiting in events | 13 | 12 | 7 |
| Press releases | 26 | 25 | 32 |

List of Media Coverage of Projects carried out between FY 2007 – 2015 (within 2 pages)

* Select main items of press releases, media coverage, and reports for FY 2007-2015 (especially by overseas media)

1) Japan

| No. | Date | Type media (e.g., newspaper, magazine, television) | Description |
|-----|----------------------------|--|---|
| 1 | 2016/2/8 - 3/8 | Nikkei, Nikkei Sangyo Shimbun, The Kahoku Shimpō | Superconducting graphene (Takahashi) |
| 2 | 2015/11/13 - 18 | Nikkan Kogyo Shinbun, Nikkei Sangyo Shimbun, Kagaku Kougyou Nippo | High Thermally Durable All-Solid-State Li Ion Battery (Orimo) |
| 3 | 2015.11.5-6 | Web news (MyNavi, Exite, Biglobe, J-Net, optronics online) | One aromatic hydrocarbon macrocycle enables a highly-efficient, phosphorescent single-layer OLEDs. (Isobe) |
| 4 | 2015/9/11 | Nikkei Sangyo Shimbun, Kagaku Kougyou Nippo | 3D Nanoporous Nitrogen-Doped Graphene with Encapsulated RuO ₂ Nanoparticles for Li-O ₂ Battery (Chen, Ito) |
| 5 | 2015/6/14 2015/2/9 - 15 | [TV] TBS "Mirai no Kigen" Nikkan Kogyo Shinbun, Nikkei Sangyo Shimbun | Ultrafine Sodium Titanate Nanowires with Extraordinary Sr Ion-Exchange Properties (Asao, Nakayama) |
| 6 | 2015/2/18 | The Kahoku Shinpo | Tohoku University Science Café (Nishiura) |
| 7 | 2014/12/12 | Science News (Kagaku Shimbun) | Anomalous superconducting states in FeSe, in collaboration (Takahashi, Tanigaki) |
| 8 | 2014/12/8 | Nikkei Sangyo Shimbun | Tohoku Univ. Supercritical Water as a catalyst (Adschiri) |
| 9 | 2014/12/2 | Nikkei Sangyo Shimbun | Success in detection of small magnetism using a metallic nanowire whose thickness is of 1/100 of a hair. Applicable to diagnosis of heart/brain diseases (Louzguine, Nakayama) |
| 10 | 2014/10/7, 8 | Nikkei Sangyo Shimbun | A feature article appeared for 2 days about the application of mathematics to materials science which Director Kotani is leading. (Kotani) |
| 11 | 2014/9/18 | Nikkei | Technology transfer to smaller companies led by Tohoku University. Technologies for reduction of friction and reuse of rare metals. (Kurihara) |
| 12 | 2014/6/10 | Web news (Nikkan Kogyo Shinbun Business Line, Asahi Shinbun Digital) | A Novel Metallic Complex Reaction Etching for Transition Metal and Magnetic Material by Low-temperature and Damage-free Neutral Beam Process for Non-volatile MRAM Device Applications (Samukawa) |
| 13 | 2013/12/14 | [TV] NHK (News) | Science Talk Live 2013 by WPI (WPI Joint Symposium) |
| 14 | 2013/10/31 | Yomiuri Shimbun, Nikkan Kogyo Shimbun | 12 centers were selected for the COI Stream (Matsue) |
| 15 | 2013/7/1 | [TV] NHK (Today's Close-up) | Learning from nature for innovation (Shimomura) |
| 16 | 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) |
| 17 | 2012/9/24 2012/9/21 | Nikkei Sangyo Shimbun Nikkan Kogyo Shimbun | World record achieved in superconducting transition temperature of transparent superconductor (Hitosugi) |

| | | | |
|----|------------------------|--|--|
| 18 | 2012/6/18 | Asahi Shimbun | NEC and Tohoku University developed a new device for generating electricity from easily-accessible heat sources. (Saitoh) |
| 19 | 2012/6/12 2012/6/11 | Nikkan Kogyo Shimbun, Kahoku Shimpō, Yomiuri Shimbun | Development of low power consumption memory (Ohno) |
| 20 | 2010/11/4 - 5 | Nikkei, Tokyo Shinbun, Asahi Shinbun, Chunichi Shinbun, Nikkan Kogyo Shinbun, Kagaku Kogyo Nippo, Asahi Shogakusei Shinbun | Japanese Scientists succeeded in photographing the image of hydrogen atoms for first time in the world. (Ikuhara) |
| 21 | 2010/7/29 | Yomiuri Shinbun, Nikkan Kogyo Shinbun | Prof. Ikuhara awarded the 2010 Humboldt Prize. The study on atomic-scale characterization and properties of interfaces in materials was evaluated. |
| 22 | 2009/9/11 | Asahi Shinbun | Showing the results of the selection of the Funding Program for World-Leading Innovative R&D on Science and Technology (Esashi) |

2) Overseas

| No. | Date | Type media (e.g., newspaper, magazine, television) | Description |
|-----|---------------------|--|---|
| 1 | 2016/2/18 - 2/23 | [Website] Build your business from our World Class Technology, HORIZON PROJECTS 2020, Graphene-info, Science Newslines Technology, AZO Nano, Graphene Uses, Science alert, PHYSICS-ASTRONOMY, Hard Science, Futurism, Asian Scientist Magazine, IEEE SPECTRUM, PHYSICS TODAY | Superconducting graphene (Takahashi) |
| 2 | 2015/5/6 - 2015/7/3 | [Website] Physics World, Yahoo News Canada, 2physics, Materials World, [Publication] Superconductor week | How to maximize the superconducting critical temperature in a molecular superconductor. (Prassides) |
| 3 | 2015/4/5 | [Website] Silicon Saxony news (Germany) | Successful cooperation of scientists of Fraunhofer ENAS and Center for Microtechnologies with the Tohoku University Sendai, Japan, in the field of micro-electromechanical systems. (Gessner, Esashi) |
| 4 | 2013/10/24 - 11/12 | [Website] Science News, Chemistry World, materials360 online | Water squishes into stable shapes, no container required (Russell) |
| 5 | 2012/2/14 | CBS News | Boston Researchers Work To Grow Human Organs (Khademhosseini) |
| 6 | 2011/6/28 | EL COMERCIO | Hay que abaratar el coste de los nanomateriales para que la sociedad los utilice (Yavari) |

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Appendix 3. List of Papers of Representative of Interdisciplinary Research Activities

* 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.

1. A. Hirata, L. J. Kang, T. Fujita, B. Klumov, K. Matsue, M. Kotani, A. R. Yavari, M. W. Chen: Geometric frustration of icosahedron in metallic glasses. **Science** 341, 376-379 (2013).

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. D. M. Packwood, S. Shiraki, and T. Hitosugi: 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 $\text{Li}_{1.3}\text{Mn}_2\text{O}_2$ 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, S. Sato, M. Kotani, H. Isobe, 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.

4. D. M. Packwood, K. T. Reaves, F. L. Federici, H. G. Katzgraber, and W. Teizer, 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. D. V. Louzguine-Luzgin, D. M. Packwood, 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 Ni₅₀Pd₃₀P₂₀ 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 $5 \times 10^{-4} \text{ s}^{-1}$, 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. 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).

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. T. Nakamura, Y. Hiraoka, A. Hirata, E.G. Escobar and Y. Nishiura, Persistent homology and many-body atomic structure for medium-range order in the glass. **Nanotechnology** 26, 304001 (2015).

The structure of glasses has been considered almost random just the same as the structure of liquid (completely molten state). However, recent studies using computational homology have revealed that there exists some short-range order in the atomic arrangement of glasses. The research team of AIMR comprising theoretical physicists, mathematicians and experimental materials scientists expanded such study to the medium-range order and discussed the relationship between the medium-range order and the short-range order. They analyzed the atomic configurations of glass materials such as silica glasses obtained by molecular dynamics simulations and suggested that “persistent diagram,” which played an important role in analyzing the short-range order of glasses, is a useful tool also to show the existence and characteristics of the medium-range order in glasses.

8. K. Inoue, M. Saito, Z.C. Wang, M. Kotani and Y. Ikuhara, The decomposition formula of <001> symmetrical tilt grain boundaries. **Materials Transactions** 56, 1945-1952 (2015).

A grain boundary is the place where two crystalline lattices having different orientations meet and shows characteristic structures depending on d-spacing of lattices and misorientation angle. An AIMR research team comprising mathematicians and experimentalists skilled in transmission electron microscopy tackled the mathematical modelling of the structures formed along grain boundaries. They used artificial boundaries formed by two single crystals attached with variety of tilt angle. The experimentalists obtained the atomic-resolution images of the symmetrical tilt grain boundaries with the tilt axis of $\langle 001 \rangle$ and the mathematicians constructed a general decomposition formula for the structures. By investigating the underlying mathematical structure, a novel algorithm to obtain the arrangement of structural units for any misorientation angle of the boundary was obtained using the Farey sequence.

9. 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).

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.

10. 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).

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.

11. M. Yan, T. Jin, Y. Ishikawa, T. Minato, T. Fujita, L.-Y. Chen, M. Bao, N. Asao, M. W. Chen and Y. Yamamoto, 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.

12. 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.

13. K. Kanetani, K. Sugawara, T. Sato, R. Shimizu, K. Iwaya, T. Hitosugi and T. Takahashi, Ca intercalated bilayer graphene as a thinnest limit of superconducting C_6Ca . **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.

14. H. Chang, Z. Sun, M. Saito, Q. Yuan, H. Zhang, J. Li, Z. Wang, T. Fujita, F. Ding, Z. Zheng, F. Yan, H.-K. Wu, M. W. Chen, and Y. Ikuhara, 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.

15. Y. Yamada, K. Ueno, T. Fukumura, H.T. Yuan, H. Shimotani, Y. Iwasa, L. Gu, S. Tsukimoto, Y. Ikuhara and M. Kawasaki, 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 TiO_2 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.

16. J.-W. Lee, Y.-C. Lin, N. Kaushik, P. Sharma, A. Makino, A. Inoue, M. Esashi and 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.)

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. S. Ahadian, J. Ramon-Azcon, M. Estili, X. B. Liang, S. Ostrovidov, H. Shiku, M. Ramalingam, K. Nakajima, Y. Sakka, H. Bae, T. Matsue, A. Khademhosseini, 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. L. Zhang, H. Chang, A. Hirata, H. Wu, Q.-K. Xue, and M. W. Chen, 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. 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 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

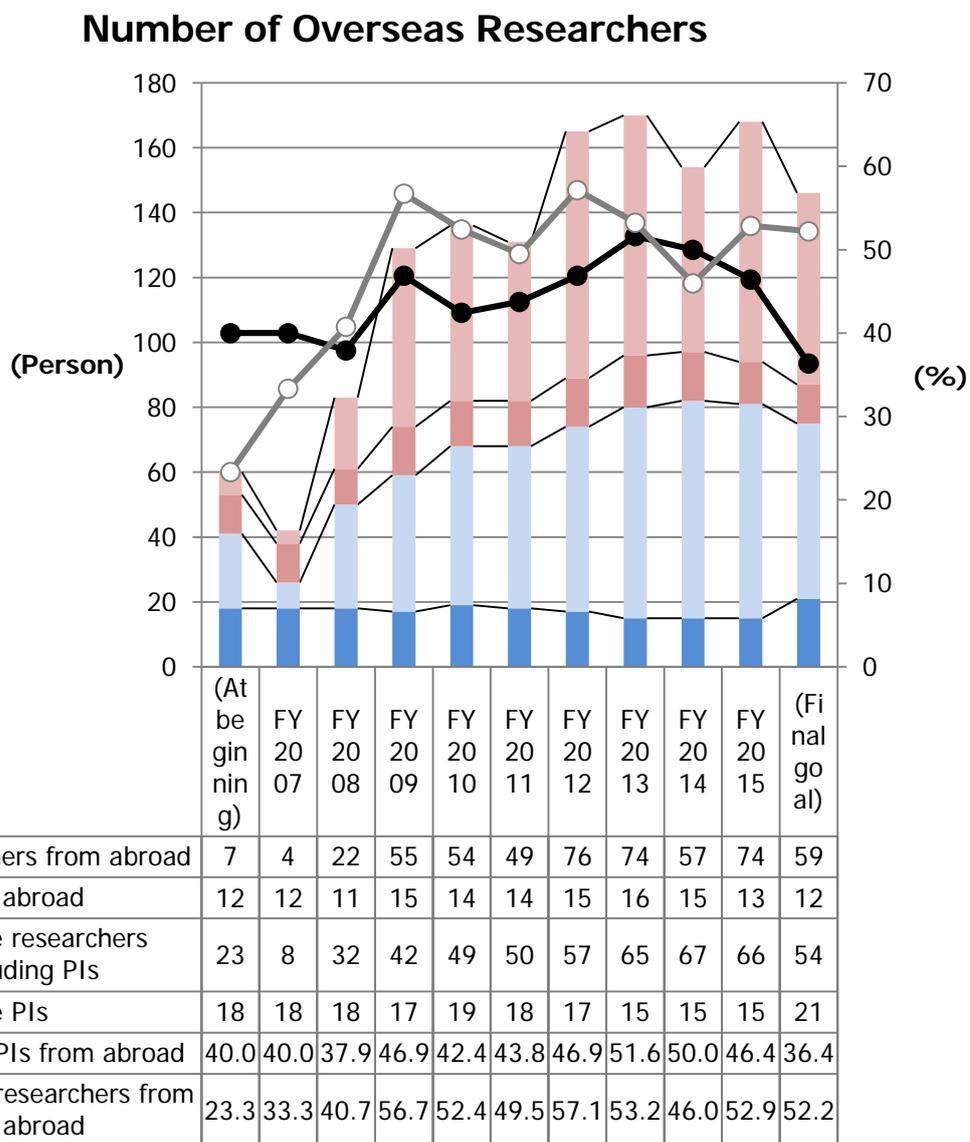
emissions with electronic switching, based on the ambipolar characteristics of organic semiconductors. Although OLETs are expected to be applied to all-organic lasers, it has so far been inhibited by a problem: the π - π stacking that boosts the mobility of charge carriers generally stifles light emissions 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).

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) Appendix 4-1. Number of Overseas Researchers and Annual Transition

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



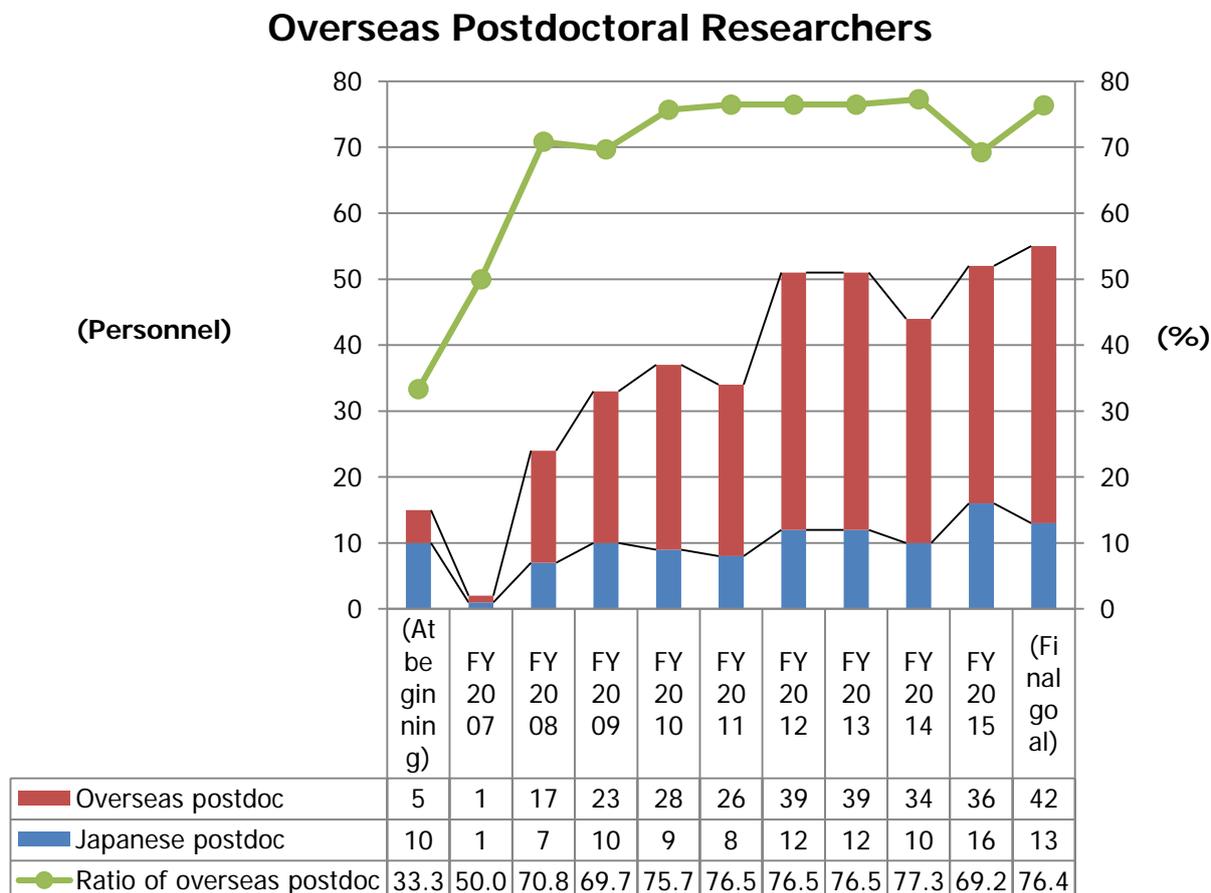
World Premier International Research Center Initiative (WPI) Appendix 4-2. Postdoctoral Positions through Open International Solicitations

- 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 %> |
| FY2014 | 156 < 154,99 %> | 3 < 3,100 %> |
| FY2015 | 116 < 114,98 %> | 3 < 2,67 %> |

World Premier International Research Center Initiative (WPI) Appendix 4-3. Number of Overseas Postdoctoral Researchers and Annual Transition

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



World Premier International Research Center Initiative (WPI)

Appendix 4-4. Status of Postdoc Employment at Institutions of Postdoctoral Researchers

*List each researcher in 1 line. If the list exceeds this form, please add extra pages.

Japanese Postdocs

| Period of project participation | Previous Affiliation Position title (Country) | Next Affiliation Position title (Country) |
|---------------------------------|---|--|
| H19.11.1~H21.2.28 | Researcher, Inst. for Materials Research, Tohoku Univ. (JPN) | Assist. Prof, Graduate School of Science, Tohoku Univ. (JPN) |
| H19.11.16~H22.3.31 | Inst. of Multidisciplinary Research for Advanced Materials, Tohoku Univ. • Researcher (JPN) | Assist. Prof., New Industry Creation Hatchery Center, Tohoku Univ. (JPN) |
| H20.4.1~H23.3.31 | Graduate School of Engineering, Univ. of Tokyo, Researcher (JPN) | Staff, Advanced Algorithm & Systems (JPN) |
| H20.4.1~H23.3.31 | Researcher, Nagoya Univ. (JPN) | Researcher, Genesis Research Inst., Inc. East Tokyo Laboratory (JPN) |
| H20.4.1~H20.12.31 | Researcher, Japan Atomic Energy Agency (JPN) | Assist. Prof., Kyushu Inst. Of Technology (JPN) |
| H20.4.1~H22.3.31 | PhD. Student, Graduate School of Engineering, Tohoku Univ. (JPN) | Researcher, TOSHIBA CORPORATION (JPN) |
| H20.4.1~H23.3.31 | Researcher, Aoyama Gakuin Univ. (JPN) | Research Assoc., Univ. of Virginia (USA) |
| H20.5.1~H23.3.31 | Researcher, Graduate School of Science, Tohoku Univ. (JPN) | Researcher, TOSHIBA CORPORATION (JPN) |
| H21.4.1~H21.12.31 | PhD. Student, The Univ. of Tokyo (JPN) | Posdoc, Kyushu Univ. (JPN) |
| H21.4.1~H23.3.31 | Research Fellowship for Young Scientists, JSPS (JPN) | Researcher, Kyushu Univ. (JPN) |
| H22.1.20~H24.3.31 | Researcher, Kyushu Univ. (JPN) | Specially Appointed Assist. Prof., Kyushu Univ. (JPN) |
| H22.4.1~H25.3.31 | PhD. Student, Graduate School of Engineering, Tohoku Univ. (JPN) | Assist. Prof., Inst. for Materials Research, Tohoku Univ. (JPN) |
| H23.4.1~H24.6.30 | PhD. Student, Graduate School of Science, Tohoku Univ. (JPN) | Staff, Hitachi Global Storage Technologies (JPN) |
| H24.4.1~H26.3.31 | Researcher, Hokkaido Univ. (JPN) | Technical Staff, Chitose Inst. Of Science and Technology (JPN) |
| H24.4.1~H25.5.31 | PhD. Student, Chuo Univ. (JPN) | Researcher, WPI-iCeMS (JPN) |
| H24.4.1~H24.7.31 | Researcher, Tohoku Univ. (JPN) | Assist. Prof., Graduate School of Engineering, Tohoku Univ. • (JPN) |
| H24.4.1~H25.9.30 | Researcher, Italian Inst. of Technology (ITA) | Waseda Univ., Assist. Prof. (JPN) |
| H24.5.1~H26.4.30 | Researcher, Osaka Univ. (JPN) | Staff, Tokyo Instruments, Inc. (JPN) |
| H24.5.1~H27.3.31 | Project Researcher, The Univ. of Tokyo (JPN) | Project Researcher, Graduate School of Arts and Sciences, the |

| | | |
|-------------------|---|--|
| | | Univ. of Tokyo (JPN) |
| H25.4.1~H28.3.31 | Specially Appointed Researcher/Fellow, Graduate School of Engineering, Osaka Univ. (JPN) | Researcher, National Inst. of Advanced Industrial Science & Technology (JPN) |
| H25.4.1~H26.3.31 | Assist. Prof., Kochi Univ. of Technology (JPN) | Assoc. Prof., Doshisha Univ. (JPN) |
| H26.8.1~H28.3.31 | Researcher, Inst. for Materials Research, Tohoku Univ. (JPN) | Researcher, Inst. for Materials Research, Tohoku Univ. (JPN) |
| H23.4.1~H24.3.31 | PhD. Student, The Univ. of Tokyo (JPN) | Research Fellowship for Young Scientists, JSPS (JPN) |
| H27.1.1~H28.3.15 | Research Fellowship for Young Scientists, JSPS (JPN) | Adjunct Associate Professor (Lecturer), Tokyo Inst. Of Technology (JPN) |
| H23.10.1~H27.9.30 | Postdoctoral Fellowship for Research Abroad, JSPS (JPN) | Assoc. Prof., Kanazawa Univ. (JPN) |
| H21.12.1~H24.8.31 | Research Fellowship for Young Scientists, JSPS (JPN) | Assist. Prof., Graduate School of Science, Tohoku Univ (JPN) |
| H20.4.1~H27.4.30 | Researcher, Inst. of Materials Structure Science, High Energy Accelerator Research Organization (JPN) | Researcher, Inst. of Physical and Chemical Research (JPN) |
| H20.4.1~H27.3.31 | PhD. Student, Graduate School of Engineering, Tohoku Univ. (JPN) | Project Assoc. Prof., Graduate School of Engineering, Tohoku Univ. (JPN) |
| H27.7.1~H27.10.31 | Technical Staff, New Industry Creation Hatchery Center, Tohoku Univ. (JPN) | Research Assoc., The Univ. of Chicago (USA) |

Overseas Postdocs

| Period of project participation | Previous Affiliation Position title (Country) | Next Affiliation Position title (Country) | Nationality |
|---------------------------------|---|--|-------------|
| H20.4.1~H20.6.30 | Researcher, Inst. for Materials Research, Tohoku Univ. (JPN) | Assist. Prof., National Univ. of Defense Technology (CHN) | CHN |
| H20.4.1~H21.6.30 | Researcher, Graduate School of Science, Tohoku Univ. (JPN) | Assist. Prof., WPI-iCeMS (JPN) | CHN |
| H20.7.1~H21.5.31 | PhD. Student, Dalian Univ. of Technology (CHN) | Postdoc, National Research Council (CAN) | CHN |
| H20.7.12~H23.3.31 | PhD. Student, Inst. of Chemistry, Chinese Academy of Sciences (CHN) | Postdoc, Inst. of Physical and Chemical Research (JPN) | CHN |
| H20.7.21~H23.12.31 | Researcher, Intl. Advanced Research Center for Power Metallurgy and New Materials (IND) | Scientist, Natl. Metallurgical Lab (IND) | IND |
| H20.8.2~H23.3.31 | PhD. Student, China Iron & Steel Research Inst. Group (CHN) | Postdoc Fellow, The Johns Hopkins Univ. (USA) | CHN |
| H20.9.11~H23.9.10 | PhD. Student, Inst. of Chemistry, Chinese Academy of Sciences (CHN) | Research Assoc., Graduate School of Pharmaceutical Science, Tohoku Univ. (JPN) | CHN |
| H20.10.20~H22.11.5 | PhD. Student, Complutense Univ. (ESP) | Researcher, Autonomas Univ. of Barcelona (ESP) | ESP |

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|---------------------|---|---|-----|
| H20.11.26~H21.8.31 | Posdoc, The Univ. of Texas at Austin (USA) | Posdoc, Chungnam National Univ. (KOR) | KOR |
| H20.12.1~H21.11.30 | Researcher, Advanced Inst. for Materials Research, Tohoku Univ. (JPN) | Assist. Prof., Univ. of Nevada (USA) | CHN |
| H21.1.14~H22.9.30 | PhD. Student, Graduate School of Engineering, Tohoku Univ. (JPN) | COE Fellow, Inst. of Fluid Science, Tohoku Univ. (JPN) | IND |
| H21.4.1~H22.3.31 | Research Assoc., Indian Inst. of Science (IND) | Staff, Department of Physics, Indian Inst. of Science (IND) | IND |
| H21.5.13~H21.8.31 | Senior Researcher, Ural State Univ. 主任研究員 (RUS) | Researcher, Inst. of Applied Acoustics (RUS) | RUS |
| H21.8.27~H25.3.31 | PhD. Student, Univ. of Science & Technology of China (CHN) | Assist. Prof., Chinese Academy of Science (CHN) | CHN |
| H21.10.1~H23.3.31 | Research Scientist, Max-Planck Inst. For Metals Research (DEU) | Prof., Inst. of Physics, Chinese Academy of Sciences (CHN) | CHN |
| H21.10.1~H23.11.25 | Posdoc, Tohoku Univ. (JPN) | Research Scientist, Inst. Of Microelectronics (SGP) | KOR |
| H21.10.29~H23.6.30 | JSPS Postdoctoral Fellowship for Foreign Researchers (JPN) | Prof., Jilin Univ. (CHN) | CHN |
| H21.11.1~H23.4.30 | Researcher, Universität Ulm (DEU) | Researcher, Leibniz Inst. for New Materials (DEU) | FRA |
| H21.11.5~H26.3.31 | PhD. Student, Changchun Inst. Of Applied Chemistry, Chinese Academy of Science (CHN) | Lecturer, Zhengzhou Univ. (CHN) | CHN |
| H21.11.15~H22.4.30 | Postdoctoral Researcher, National Inst. for Materials Science (JPN) | Assist. Prof., Inst. of Metal Research, China Academy of Sciences • (CHN) | CHN |
| H22.1.12~H24.3.31 | Researcher, Tohoku Univ. (JPN) | JSPS Postdoctoral Fellowship for Foreign Researchers (JPN) | BRA |
| H22.1.25~H23.3.31 | Posdoc, Univ. of Alabama (USA) | Returned to home country | IND |
| H22.3.16~H23.3.31 | Assist. Prof., College of Engineering, King Saud Univ. (SAU) | Assist. Prof., Graduate School of Science, Tohoku Univ. (JPN) | BGD |
| H22.3.24~H23.4.12 | Postdoctoral Staff Researcher, Toyota Technical Center, Materials Research Department (USA) | Researcher, North Carolina State Univ. (USA) | USA |
| H22.4.1~H23.2.15 | Project Researcher, Graduate School of Medicine, The Univ. of Tokyo (JPN) | Technical Staff, Okinawa Inst. Of Science & Technology Graduate Univ. (JPN) | IRN |
| H22.4.1~H23.2.28 | Research Assist., Max-Planck Inst. For Solid State Research (DEU) | Posdoc, Inst. of Physical and Chemical Research (JPN) | DEU |
| H22.6.24~H22.12.24 | Assist. Prof., Inst. Of Semiconductors, Chinese Academy of Sciences (CHN) | Assist. Prof., Inst. Of Semiconductors, Chinese Academy of Sciences (CHN) | CHN |
| H22.7.12~H25.3.31 | Assist. Prof., Tianjin Polytechnic Univ. (CHN) | Assist. Prof., Tianjin Polytechnic Univ. (CHN) | CHN |
| H22.11.1~H25.3.31 | PhD. Student, Chinese Academy of Sciences (CHN) | Assist. Prof., Univ. of Wisconsin (USA) | CHN |
| H22.11.24~H26.11.23 | Researcher, CNRS (FRA) | Returned to home country | FRA |
| H22.12.1~H23.8.31 | Research Assoc., The University of Melbourne (AUS) | Posdoc Research Fellow, Aarhus Univ. (DNK) | SGP |

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|--------------------|---|--|-----|
| H22.12.1~H25.3.31 | Senior Researcher, National Univ. of Science & Technology (MISIS)(RF) | Research Assoc., Scientific and Research Center of Composite Materials of the National Univ. of Science and Technology MISIS (RUS) | RUS |
| H23.1.18~H24.5.31 | Researcher, Univ. of Texas (USA) | Assoc. Prof., Shanghai Inst. of Material Medica, Chinese Academy of Sciences (CHN) | CHN |
| H23.2.1~H23.10.31 | Posdoc, National Inst. for Materials Science (JPN) | JSPS Postdoctoral Fellowship for Foreign Researchers (JPN) | CHN |
| H23.7.1~H25.6.30 | PhD. Student, Inst. of Chemistry, Chinese Academy of Sciences (CHN) | Researcher, Ulsan National Inst. of Science and Technology (KOR) | CHN |
| H23.7.1~H25.8.31 | PhD. Student, Shandong Univ. (CHN) | Teacher, Southwest Petroleum Univ. in Sichuan Province (CHN) | CHN |
| H23.7.14~H27.3.23 | PhD. Student, Inst. of Physics, Chinese Academy of Sciences (CHN) | Posdoc, Johns Hopkins Univ. (USA) | CHN |
| H23.10.1~H24.3.31 | PhD. Student, Hong Kong Univ. of Sci. & Tech. (CHN) | Assoc. Prof., Sun Yat-sen Univ. (CHN) | CHN |
| H24.1.1~H26.7.31 | Researcher, Micro System Integration Center, Tohoku Univ. (JPN) | Researcher, MEMS CORE Co., Ltd. (JPN) | TWN |
| H24.2.1~H24.3.31 | Researcher, UCL (GBR) | Research Assoc. UCL (GBR) | CHN |
| H24.2.3~H26.3.31 | Postdoctoral Research Fellow, McMaster Univ. (CAN) | Assist. Prof., Inst. of Technology Bandung (IDN) | IDN |
| H24.4.1~H26.4.30 | PhD. Student, Nagoya Univ. (JPN) | Returned to home country | IND |
| H24.5.1~H25.3.31 | Researcher, Pusan National Univ. (KOR) | Researcher, Inst. of Multidisciplinary Research for Advanced Materials, Tohoku Univ (JPN) | KOR |
| H24.9.1~H26.3.31 | PhD. Student, Nankai Univ. (CHN) | Research Fellow, Nanyang Technology Univ (SGP) | CHN |
| H24.9.1~H27.2.28 | PhD. Student, Donghua Univ. (CHN) | Researcher, Ningbo Inst. of Industrial Technology, CAS / Ningbo Fu materials Co. Ltd. (CHN) | CHN |
| H24.9.16~H28.3.31 | PhD. Student, Pisa Univ. (ITA) | Researcher, Kyushu Univ. (JPN) | VNM |
| H24.10.9~H27.1.31 | PhD. Student, Tampere Univ. of Technolog ((FIN) | Science Fellow, Aalto Univ. (FIN) | ITA |
| H24.11.3~H25.11.2 | Researcher, Univ. of Cambridge (GRB) | Research Associate, The Univ. of Cambridge (GBR) | CZE |
| H24.12.1~H26.9.15 | PhD. Student, Technische Universität Berlin (DEU) | Chemist, BASF-the Chemical company (DEU) | FRA |
| H24.12.1~H25.11.30 | Researcher, Nanoco Technologies Ltd. (GRB) | Research Associate, The Univ. of Cambridge (GBR) | GBR |
| H25.1.15~H26.1.14 | JSPS Postdoctoral Fellowship for Foreign Researchers (JPN) | Posdoc Research Fellow, National Inst. for Materials Science (JPN) | CHN |
| H25.3.18~H26.12.31 | Researcher, Univ. of California, Santa Barbara (USA) | Posdoc, Rice Univ. (USA) | CHN |

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|--------------------|--|--|-----|
| H25.4.1~H27.3.31 | Researcher, Research Inst. of Electrical Communication, Tohoku Univ. (JPN) | Posdoc, Regensburg Univ. (DEU) | CHN |
| H25.7.26~H26.7.25 | PhD. Student, Aix-Marseille Univ. (FRA) | Returned to home country | FRA |
| H25.10.1~H27.8.30 | PhD. Student, Peking Univ. (CHN) | Lecturer, North China Electric Power Univ. (CHN) | CHN |
| H25.10.3~H27.1.31 | Researcher, Inst. for Energy Technology (NOR) | Research Assoc., Curtin Univ. (AUS) | GBR |
| H25.11.1~H26.7.31 | PhD. Student, Univ. of Zurich (CHE) | Research Scientist, (The company will start in September in Swiss) (CHE) | ITA |
| H26.4.1~H27.10.31 | PhD. Student, Graduate School of Science, Tohoku Univ. (JPN) | Researcher, Tokyo Inst. Of Technology (JPN) | CHN |
| H26.4.1~H28.3.31 | PhD. Student, Graduate School of Engineering, Tohoku Univ. (JPN) | Researcher, Inst. for Materials Research, Tohoku Univ. (JPN) | CHN |
| H27.1.1~H27.9.30 | PhD. Student, Graduate School of Engineering, Osaka Univ. (JPN) | Specially Appointed Assist. Prof., Osaka Univ. (JPN) | VNM |
| H27.4.1~H28.2.29 | Posdoc, Universite Lille Nord de France, CNRS (FRA) | Assist. Prof., Changchun Inst. Of Applied Chemistry, Chinese Academy of Science (CHN) | CHN |
| H23.4.2~H27.6.30 | PhD. Student, Graduate School of Engineering, Tohoku Univ. (JPN) | Research Fellow, Univ. of Toronto (CAN) | IRN |
| H23.4.1~H26.4.30 | Researcher, Univ. of Hyogo (JPN) | Assist. Prof., Inst. of Advanced Chemistry of Catalonia (IQAC) at Spanish Council for Scientific Research (CSIC) (ESP) | ESP |
| H20.5.1~H27.9.25 | Research Scientist, Honey Well Company (USA) | Prof., Beijing Univ. (CHN) | CHN |
| H22.10.14~H27.2.28 | PhD. Student, South CHN Univ. of Technology (CHN) | Prof., South China Univ. of Technology (CHN) | CHN |
| H23.2.15~H26.7.22 | Researcher, The Hong Kong Polytechnic Univ. (HKG) | Prof., Huazhong Univ. of Science and Technology (CHN) | CHN |
| H22.4.1~H26.10.31 | Posdoc, Inst. for Materials Chemistry and Engineering, Kyushu Univ. (JPN) | Prof., Northeastern Univ. of China (CHN) | CHN |
| H20.9.1~H26.3.31 | PhD. Student, Tsinghua Univ. (CHN) | Research Associate Prof., School of Materials Science and Engineering, Tsinghua Univ (CHN) | CHN |
| H19.12.13~H27.7.31 | Research Lecturer, School of Electronics Engineering, Korea Univ. (KOR) | Prof., East China Univ. of Science & Technology (CHN) | CHN |

World Premier International Research Center Initiative (WPI)

Appendix 4-5. 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

2. **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 PREMIER 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:** 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

4. **Counterpart of an Agreement:** Institute of Chemistry, Chinese Academy of Sciences
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 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

5. **Counterpart of an Agreement:** Department of Chemistry, University of Cambridge
Name of an Agreement: AGREEMENT ON ACADEMIC EXCHANGE BETWEEN THE WORLD PREMIER INTERNATIONAL RESEARCH CENTER ADVANCED INSTITUTE FOR MATERIALS RESEARCH (WPI-AIMR) TOHOKU UNIVERSITY, JAPAN AND DEPARTMENT OF CHEMISTRY 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

6. **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

7. **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

8. **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
9. **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
10. **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
11. **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

- 12. 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
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
- 13. 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
- 14. 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
- 15. 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
- 16. 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
- 17. 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

18. 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

World Premier International Research Center Initiative (WPI)

Appendix 4-6. Holding International Research Meetings

* For each fiscal year, indicate the number of international research conferences or symposiums held and give up to two examples of the most representative ones using the table below.

| Date | Meeting title and Place held | Number of participants |
|---|---|------------------------|
| February 21 st – 24 th , 2016 | The AIMR International Symposium 2016 (AMIS2016) (Sendai, Japan) | 235 |
| November 27 th – December 3 rd , 2015 | Eighth French Research Organizations - Tohoku University Joint Workshop on Frontier Materials (Sendai, Japan) | 100 |
| November 13, 2015 | Tohoku University - IMEC Seminar 2015 (Sendai, Japan) | 80 |
| February 16 th – 19 th , 2015 | The AIMR International Symposium 2015 (AMIS2015) (Sendai, Japan) | 268 |
| October 19 th -21 st , 2014 | International Symposium on the Synthesis and Application of Curved Organic π - Molecules and Materials (Kyoto, Japan) | 150 |
| June 25 th -27 th , 2014 | 12th RIEC International Workshop on Spintronics (Sendai, Japan) | 100 |
| May 26 th -27 th , 2014 | JSPS 141 Committee Award (Sendai, Japan) | 100 |
| February 16 th – 19 th , 2014 | The AIMR International Symposium 2014 (AMIS2014) (Sendai, Japan) | 236 |
| November 22 nd , 2013 | AIMR/UCL Materials Workshop (London, UK) | 50 |
| 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 | The 2 nd AIMR-CNSI workshop (Sendai, Japan) | 52 |
| 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 | The 2012 WPI-AIMR Annual Workshop (Sendai, Japan) | 267 |
| January 9 th -13 th , 2012 | UCSB ICMR/CNSI and Tohoku University WPI-AIMR Joint Workshop on Materials Research (Santa Barbara, USA) | 34 |
| November 24 th -26 th , 2011 | New Science Created by Materials with Nano Spaces: From Fundamentals to Applications (Sendai, Japan) | 100 |
| 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 | 80 |
| March 1 st -6 th , 2009 | The 2009 WPI-AIMR Annual Workshop (Zao, Miyagi, Japan) | 180 |
| | | |
| | | |
| | | |
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| | | |

World Premier International Research Center Initiative (WPI)

Appendix 5-1. Host Institution's Commitment

1. Contributions from host institution

(1) Fund, Personnel

* Regarding "Fund" entry, describe with reference to the items in the Progress Report (Jisseki-hokoku-sho) based on Article 12 of the Grant Guidelines (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.

| (2007-2012) | | | | | | |
|--|-------|---------|--------|---------|---------|---------------|
| <Fund> | | | | | | (million yen) |
| Fiscal Year | 2007 | 2008 | 2009 | 2010 | 2011 | 2012 |
| Personnel | 11 | 164 | 243 | 24 | 75 | 257 |
| - Faculty members (including researchers) | | | | | | |
| Full-time | | 94 | 130 | 19 | 3 | 188 |
| Concurrent | 9 | | | | | |
| Postdocs | | | | | | |
| RA etc. | | | | | | |
| Research support staffs | | 1 | 24 | | | |
| Administrative staffs | 2 | 69 | 89 | 5 | 72 | 69 |
| Project activities | 5 | 101 | 105 | 116 | 122 | 53 |
| Travel | 0 | 8 | 7 | 1 | 0 | 8 |
| Equipment | 0 | 932 | 161 | 0 | 61 | 30 |
| Research projects | 350 | 599 | 204 | 193 | 30 | 18 |
| Total | 366 | 1,804 | 720 | 334 | 288 | 366 |
| <Personnel> | | | | | | (person) |
| Fiscal Year | 2007 | 2008 | 2009 | 2010 | 2011 | 2012 |
| Personnel | | | | | | |
| - Faculty members (including researchers) | 2 | 15 | 14 | 16 | 3 | 18 |
| Full-time | | 13 | 12 | 15 | 3 | 16 |
| Concurrent | 2 | 2 | 2 | 1 | | 2 |
| Postdocs | | | | | | |
| RA etc. | | | | | | |
| Research support staffs | | 2 | 12 | | | |
| Administrative staffs | 1 (0) | 12 (11) | 24(11) | 12 (12) | 17 (16) | 10 (10) |

| (2013-2016) | | | | | |
|--|-------------|----------------------|-------------|-------------|--------------|
| <Fund> | | (million yen) | | | |
| Fiscal Year | 2013 | 2014 | 2015 | 2016 | Total |
| Personnel | 242 | 197 | 264 | 259 | 1,736 |
| - Faculty members (including researchers) | | | | | |
| Full-time | 177 | 125 | 170 | 181 | 1,087 |
| Concurrent | | | | | 24 |
| Postdocs | | | | | |
| RA etc. | | | | | |
| Research support staffs | 1 | | 11 | | 37 |
| Administrative staffs | 64 | 72 | 68 | 78 | 588 |
| Project activities | 3 | 24 | 23 | 23 | 575 |
| Travel | 1 | 0 | 3 | 9 | 37 |
| Equipment | 39 | 30 | 35 | 13 | 1,271 |
| Research projects | 38 | 31 | 47 | 35 | 1,545 |
| Total | 323 | 282 | 342 | 339 | 5,164 |
| <Personnel> | | (person) | | | |
| Fiscal Year | 2013 | 2014 | 2015 | 2016 | Total |
| Personnel | | | | | |
| - Faculty members (including researchers) | 19 | 18 | 23 | 21 | 149 |
| Full-time | 17 | 16 | 21 | 19 | 132 |
| Concurrent | 2 | 2 | 2 | 2 | 17 |
| Postdocs | | | | | |
| RA etc. | | | | | |
| Research support staffs | 1 | | 12 | 12 | 39 |
| Administrative staffs | 10 (10) | 10 (10) | 13 (12) | 13 (12) | 122 (104) |

(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. In addition, outward facilities of the AIMR Main Building including a parking area for bicycles were constructed in FY2015 and provided for the Center. 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.

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. In order to strengthen this system further, the head of the host institution, the President of Tohoku University, pledged to prepare additional 10 tenure positions for the Center. As the first example utilizing the positions, the Center invited a professor from Durham University, U.K., and he became a full professor of the Center in FY2014. The second one was that one existing junior PI was promoted to PI via international recruitment also in FY2014. As the third one, one researcher was employed from outside of the Center and appointed to junior PI in FY2015. As the official department, the Center is involved in the self-evaluation of the departments within the host institution and this enables the Center to obtain the allocation of resources such as the university's operational funds, discretionary funds of the president, and funds for the promotion of university reform and established the budgetary basis for the operation of the Center.

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 has acted as adviser to the Center Director from the standpoint of the entire university. In addition, in FY2015, a new personnel scheme gathering excellent researchers through the cooperation between the

Center and related departments was introduced based on the proposal by the host institution.

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. Furthermore, the host institution held the workshop for the office staff of the entire university to encourage them to understand the international office works and increase their motivation to learn English; the speakers at the workshop were from the administrative office of the Center. 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 have been continuously distributed to all administrative staff in the host institution from FY2014. In addition, the host institution has established International Affairs Center (IAC) in the Organization for Advanced Studies in FY2015 to strengthen the support for foreign researchers and is preparing for the new stage after the termination of the WPI's financial support.

5. 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.

6. Support for other types of assistance

Other than those above, the host institution stipulated support for the Center and strengthening of the Center in the first, second and third period of the "Mid-term Plan" of Tohoku University. The host institution will provide the Center full support as the first institute involved in "WPI-type special ward, Organization for Advanced Studies" which was established by Tohoku University's Global Initiative (selected by MEXT's Top Global University Project) in FY2014 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.

World Premier International Research Center Initiative (WPI)

Appendix 5-2. The Host Institution's Mid-term Plan

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. 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 University and the world's top overseas universities, including invitation of researchers from said universities.

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.

World Premier International Research Center Initiative (WPI)

Appendix 5-3. Transition in the Number of Female Researchers

* Enter the number and percentage of female researchers in the top of each space from 2010 to 2015 and the total number of all the researchers in the bottom.

(person)

| | FY2010 | FY2011 | FY2012 | FY2013 | FY2014 | FY2015 | Final goal |
|----------------------------|---------|---------|---------|---------|---------|---------|------------|
| Researchers | 14,10 % | 11, 8 % | 15, 9 % | 16, 9 % | 10, 6 % | 15, 9 % | 22,15 % |
| | 136 | 131 | 165 | 170 | 154 | 168 | 146 |
| Principal investigators | 2, 6 % | 2, 6% | 2, 6 % | 2, 6% | 2, 7 % | 2, 7 % | 2, 6 % |
| | 33 | 32 | 32 | 31 | 30 | 28 | 33 |
| Other researchers | 12,12 % | 9, 9 % | 13,10 % | 14, 10% | 10, 8% | 13, 9 % | 20,18 % |
| | 103 | 99 | 133 | 139 | 124 | 140 | 113 |

World Premier International Research Center Initiative (WPI) Progress Plan (For Final Evaluation)

| | | | |
|------------------|--|-----------------------|---------------|
| 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 6 pages**.

* Use yen (¥) when writing monetary amounts in the report. If an exchange rate is used to calculate the yen amount, give the rate.

1. Mid- to Long-term Research Objectives and Strategies Based on the Center's Results during Funded Period

Describe new challenges in the Center's research objectives and plans after the funding period ends. If major adjustments will be made in the Center's operation, such as newly set research themes/objectives or a change in the director, describe the strategic background to the adjustments.

AIMR aims to create new materials with innovative functions that contribute to society by building a foundation for safe and enriched livelihoods, conducted by a world-leading organization for interdisciplinary research. Excellent researchers from around the world continuously produce high-quality results. Their research has been evaluated yearly as "world-leading" by the WPI Program Committee, as well as by international scientific communities. In the FY2011 Interim Evaluation, AIMR clarified its identity "discovering commonalities and universal principles among different fields and creating new materials science that predicts new functions and structures producing such functions" by integrating mathematics to articulate objectives and accelerate initiatives. After the Interim Evaluation, under the leadership of new Center Director Motoko Kotani, AIMR rapidly re-organized to initiate the mathematics-materials science collaboration with a Mathematics Unit, Interface Unit, and three Target Projects. AIMR cleared the two-year careful observation with "remarkable progress beyond expectations." In the Extension Application Screening carried out in FY2014, AIMR was accounted to have achieved "World Premier Status" based on the top world-level materials science produced by the mathematics-materials science collaboration.

After the termination of the ten-year support by WPI program, AIMR will maintain its organization and management system, flexibly and rapidly implementing strategy to address the most recent scientific topics; and to maintain a "world-class" research environment with excellent researchers from around the world. AIMR will create new materials science appropriate for the 21st century with mathematics-materials science collaboration. AIMR will focus on the following areas, based on the strengths it has developed in the past years.

1) Spin-centered materials science: Discussing the "physics of spin current" has become a reality through recent development of theories and technologies, and opportunities have emerged for changing conventional charge current-centered physics and developing new technologies based on recent spin physics. We have succeeded in creating microscopic non-dissipative phenomena using spin, facilitating a new theoretical principle to control energy and information transfer with mathematical guidance. This will stimulate fundamental theoretical developments in mathematics and physics and expand AIMR-pioneered technologies, such as

energy saving devices using "tunnel magnetoresistance" and "magnetic semiconductors," and new power generation system using the "spin Seebeck effect."

2) Design of hierarchical structure based on theoretical prediction: At AIMR, by clarifying our objectives at establishment, target projects have been pursued to build the basis for materials science where material properties can be predicted. We have revealed interaction among the layers of hierarchy and the relationship between the dynamic structure formation of non-equilibrium systems and functions through the introduction of mathematical indices. Based on these new findings, we will provide indices of guiding principles to find new structures, and create the pattern formation model for realization of the proposed structures and develop theories to evaluate stability with numerical validation. With a view to the construction of "Topological Design" that enables calculations for predicting the properties of materials based on "computational homology," we will build the foundation for enabling the smart design of materials within a mathematical framework.

With respect to the organizational framework for research, Tohoku University has established the "Organization for Advanced Studies" in FY2014 based on AIMR, putting AIMR as the first institute in the organization. Also included are the "Tohoku Forum for Creativity" which invites world authorities for medium term programs, the international administrative office, and the research reception center. The "Graduate School of Spintronics (Graduate Program in Spintronics (GP-Spin))," where AIMR researchers are core members, has been established, bringing world-leading researchers and excellent graduate students to Tohoku University. AIMR and AIMR researchers will play a central role in all of these, leading Tohoku University in reinforcing research and globalization. With respect to overseas expansion, AIMR will maintain the international partnership with the existing satellites. Based on these, as a long-term objective, AIMR will flexibly and quickly develop a strategy as a world leader in materials science, contributing to society by creating revolutionary functional materials based on new materials science born at AIMR.

Following are details of the challenges AIMR will continuously tackle even after the termination of the support by WPI program to advance AIMR as a world-leading institute.

(1) Reaching maturity in mathematics-materials science collaboration and creation of new materials science based on it

Materials science has been a strong point of Japan, not only in science and technology, but also in economics in the international community. However, materials research is at a turning point when considering, for instance, the rapid advancement of China; and the "Materials Genomics Initiative" (MGI) in the United States that utilizes the information and communication technology (ICT). Under those circumstances, AIMR's pioneering approach for building a mathematical foundation to predict complicated functional expressions of materials is quite timely in putting forth highly-functional numerical calculations for predictive capabilities of materials properties. On the other hand, in mathematics, many recent Fields medalists are researchers in mathematical physics, where they construct mathematical theories dealing with physics problems. The 2011

Kyoto Prize (Advanced Technology) was awarded to Dr. John Werner Cahn, who established the mathematical model of phase separation of materials; and in 2014 the physicist Dr. Edward Witten was awarded the Kyoto Prize (Basic Sciences, Mathematical Science), indicating that mathematics and physics have already united. The latest topological materials and quantum materials fully utilize very recent profound mathematics such as Index Theorems and Noncommutative Geometry; and offer challenges on the frontier of materials science that appeal to mathematicians. Materials science offers important challenges that lead advancements on the frontier of mathematics, while mathematics has matured to a level that can deal with complex materials science. The foundation for a mutual relationship in mathematics and materials science is now emerging.

AIMR set three target projects, "*Non-equilibrium Materials based on Mathematical Dynamical Systems*", "*Topological Functional Materials*", and "*Multi-Scale Hierarchical Materials based on Discrete Geometric Analysis*," and made a system in which experimental results from leading experimental scientists and predictions from mathematical models can interactively stimulate each other. As a result, research themes have been identified which stimulate both materials researchers and mathematicians. We will focus on these and achieve breakthroughs in the two fields mentioned above, "**Spin-centered materials science**" and "**Design of hierarchical structure based on theoretical prediction.**" We will focus on new mathematical theories describing the global structure of amorphous materials, constructing new physics centered upon "spin," quantization of surface and interface states through Noncommutative Geometry and Index Theorems, and create a new theory for dynamic systems of highly dense nanoparticle systems with a hybrid algorithm of Phase-Field Method (PFM) and fluid equations.

It has been pointed out recently that it is crucial to rationalize design and development of materials and tighten the development cycle by constructing a database of research results related to materials science, and analyzing Big Data from Informatics Theory and Mathematics. However, simply applying informatics methods is not enough to meet this challenge. It is essential that the best experimental materials scientists, theoretical physicists, and mathematicians repeatedly interact under one roof, thoroughly understand the mechanism of function expressions, extract the appropriate mathematical concepts, and develop mathematical models. Along these lines, AIMR has already produced some promising results within a short period, with full potential to bring about a paradigm shift. We plan to construct a new materials informatics method enabling *molecular simulations* and *time-series analysis of high-dimensional phase information*, interactively based upon a *homological database* for predicting materials' properties by a combination of *topological analysis* and *data-driven methods*.

AIMR's leading activities that aim to create predictive materials science based on mathematical principles appropriate for the 21st century have been recognized in the international mathematics community, as evidenced by the publication in "SpringerBriefs in the Mathematics of Materials" (Editor-in-Chief M. Kotani) and, in Asian Foresight, of "Modeling and Simulation of Hierarchy and Heterogeneous Flow systems with Applications to Materials Science" (PL Y. Nishiura).

(2) Maintaining the international partnership

For AIMR to lead the world by creation of new materials science, it is necessary to keep the international partnership that AIMR have constructed until now and it is important to maintain the cooperative relationship with the existing satellites. AIMR will maintain the strong relationship with five institutions shown in **Appendix 2**, the University of Cambridge, the University of California, Santa Barbara (including the partnership with CNSI and IPAM, UCLA), Beijing (Tsinghua University and Chinese Academy of Sciences), Chemnitz University of Technology (Fraunhofer ENAS; we are operating the AIMR-Fraunhofer Project Center at AIMR), and the University of Chicago.

The superiority of AIMR in such international partnerships is realized in the mathematics-materials science collaboration first pioneered by AIMR. The importance of cooperation between various fields and mathematics, which serves as the bedrock for innovation, has been repeatedly noted and reflected in President Obama's support for mathematics in the United States; and the global trend of mathematics cooperating with other fields is clearly progressing. In this movement, bringing the mathematics-materials science collaboration pioneered by AIMR into the global arena is a response to global demands. AIMR has started a global trend and is becoming a world leader.

2. Management System of the Research Organization

2-1. Describe the Center's Research Organizational Management System that will Execute the Research Strategy and Plan Described above.

- In Appendix 1, list the PIs who will ensure that the Center's project is sustained and advanced after the funding period ends.
- In Appendix 2, diagram the Center's organizational management system.

Center Director Motoko Kotani and PIs listed in **Appendix 1** will be united, pursuing pioneering research. As shown in **Appendix 2**, the Center's management organization system follows the present system with five research groups, "Materials Physics," "Non-equilibrium Materials," "Soft Materials," "Device/System," and "Mathematical Science." The top-down management by the Center Director and a global standard research environment (including the merit-based salary system), as well as a support system will also be maintained. The Center is managed with flexibility and quick decision-making. The joint appointment system will further promote personnel exchange between AIMR and research groups in the university, and inside and outside Japan. In particular, we will establish a career path for young researchers by making a tenure-track system based on organic networking with other university departments.

With respect to the organization for internationalization, AIMR will maintain the international partnership with the University of Cambridge, the University of California, Santa Barbara (and UCLA), Beijing, Chemnitz University of Technology (Fraunhofer ENAS), and the University of Chicago.

2-2. Initiatives and Plans that will Impel System Reforms

Describe the Center's action plan that embodies the basic policies of the National University Reform Plan or Independent Administrative Agency Reform Plan, and the Center's plan and strategies that lead to host institution reforms either directly or via ripple effects (also to other institutions, if applicable). Describe also the Center's strategies for fostering and securing the next generation of researchers (e.g., introduction of tenure tracks), and the system for enhancing the Center's organizational management, such as the implementation/verification PDCA system.

Tohoku University established the president's action plan "SATOMI VISION," pursuing organizational and system reform to realize the "creation of an international community of knowledge." While reinforcing research according to world standards, internationalization, and system reform, Tohoku University is preparing to bring AIMR measures to the entire university.

In FY2014, Tohoku University established the "Organization for Advanced Studies" modeled upon AIMR's internationalization and system reform to construct an international research environment and support system that gathers world-leading researchers at Tohoku University and creates new scientific disciplines exceeding existing ones, putting AIMR first in the organization (see **Appendix 3**). This is a central point of the university's plan to realize resource redistribution and personnel management system reform. Independent, top-down decision-making by the institute directors, merit-based salaries, internationalization (ratio of overseas researchers and English services), and a research support system will be or partially have been introduced into the organization, based on AIMR. Also to have been incorporated are the international administrative office and the research reception center (providing services for inviting overseas researchers) after expanding AIMR's Administrative Division, and "Tohoku Forum for Creativity" which will inherit and upgrade the "GI³ Laboratory Program," which has been the driving force for holding international meetings and inviting researchers from abroad. Online procedures for obtaining a visa and systematizing the support system for international activities, such as support for invitations, will be established; and all systems will become more flexible.

Moreover, university administrative system reform, based on AIMR, entails a "establishment of a Promotion Office for operation reform" and "an administrative system providing services in English throughout the university." Along with the report by "Working Group for a Flexible Personnel Management System," a "joint appointment system" will be set up based on AIMR, facilitating the invitation of researchers. An annual salary employment system with merit-based salaries will be expanded or reexamined, accelerating employment of excellent researchers. The "Industrial-Academic Partnership Project" (first established by AIMR) has also commenced.

3. Center's Position within Host Institution and Measures to Provide It Resources

Describe the Center's future plans with regard to the following points after the funding period ends.

3-1. From a Mid- to Long-term Perspective, the Position of the Center within the Organization of the Host Institution

Describe where the Center will be placed within the host institution's overall organizational strategy under the leadership of the institution's president.

- In Appendix 3, diagram the Center's position within the organization of the host institution, and describe that positioning using excerpts from the institution's mid- to long-term plan. If the plan has not been established yet, describe the consideration being given to the Center's positioning.

Statements regarding AIMR's position in Tohoku University's "Third Mid-term plan" are shown in **Appendix 3**, where promoting AIMR is one of its most important parts. AIMR was established as an official university department where Tohoku University placed tenured faculty and permanent administrative staff at AIMR. Tohoku University will maintain AIMR as a top-level research center leading the university's plans for "establishing world-leading research institutes"

and to “jump to world class as the hub of global brain circulation,” as stipulated in SATOMI VISION, even after WPI program support ends. As shown in **Appendix 3**, Tohoku University established the “Organization for Advanced Studies” in FY2014 directly under the President, putting AIMR first.

3-2. Host Institution’s Action Plan for Sustaining and Advancing the Center as a World Premier International Research Center (e.g., positioning, financial resources)

The resource plan is shown in **Appendix 4**. President Satomi pledged to keep permanent staff members (16 proper (tenure) faculties and 10 administrative staff) already placed at AIMR, and add 10 tenure positions. The five of the ten positions have been occupied by Prof. Kosmas Prassides (PI), Prof. Shigemi Mizukami (PI), Prof. Yasuaki Hiraoka (PI), Prof. Ayumi Hirano (PI) and Assoc. Prof. Hiroshi Yabu (tenure-track Junior PI). The other remaining positions will be gradually offered via international recruitment. The financial resource from the host institution will be used mainly to start the laboratories of such tenure positions and to keep young researchers of Mathematical Science Group and staff of the international administrative office. Part of the resource will also be used to maintain cooperative relationship with the overseas satellites as mentioned above. It is necessary to maintain research and international activities by keeping at least two thirds of the present scale (especially the number of young researchers) of the Center in order for AIMR to keep a position as the world leader to create new materials science based on mathematics-materials science collaboration. We will make maximum effort to keep young experimental researchers (assistant professors and postdoctoral researchers) by using external sources.

World Premier International Research Center Initiative (WPI)

Appendix 1. List of Principal Investigators for Progress Plan

- If the number of principal investigators exceeds 10, add columns as appropriate.
- Place an asterisk (*) by the name of the investigators who are considered to be ranked among the world's top researchers.
- Give age as of 1 April 2017
- For investigators who cannot participate in the center project from its beginning, indicate the time that their participation will start in the "Notes" column.

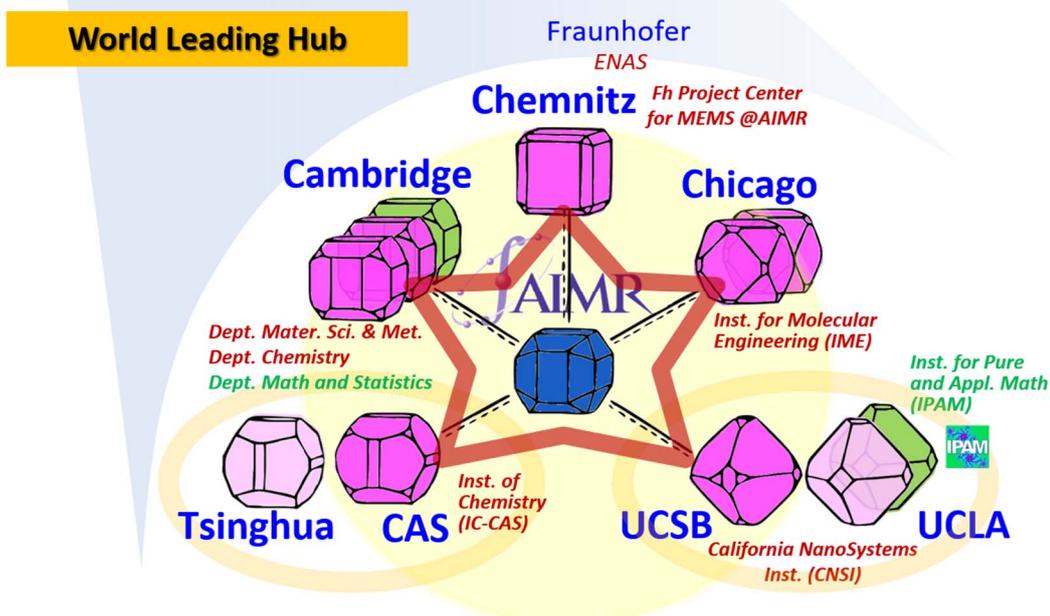
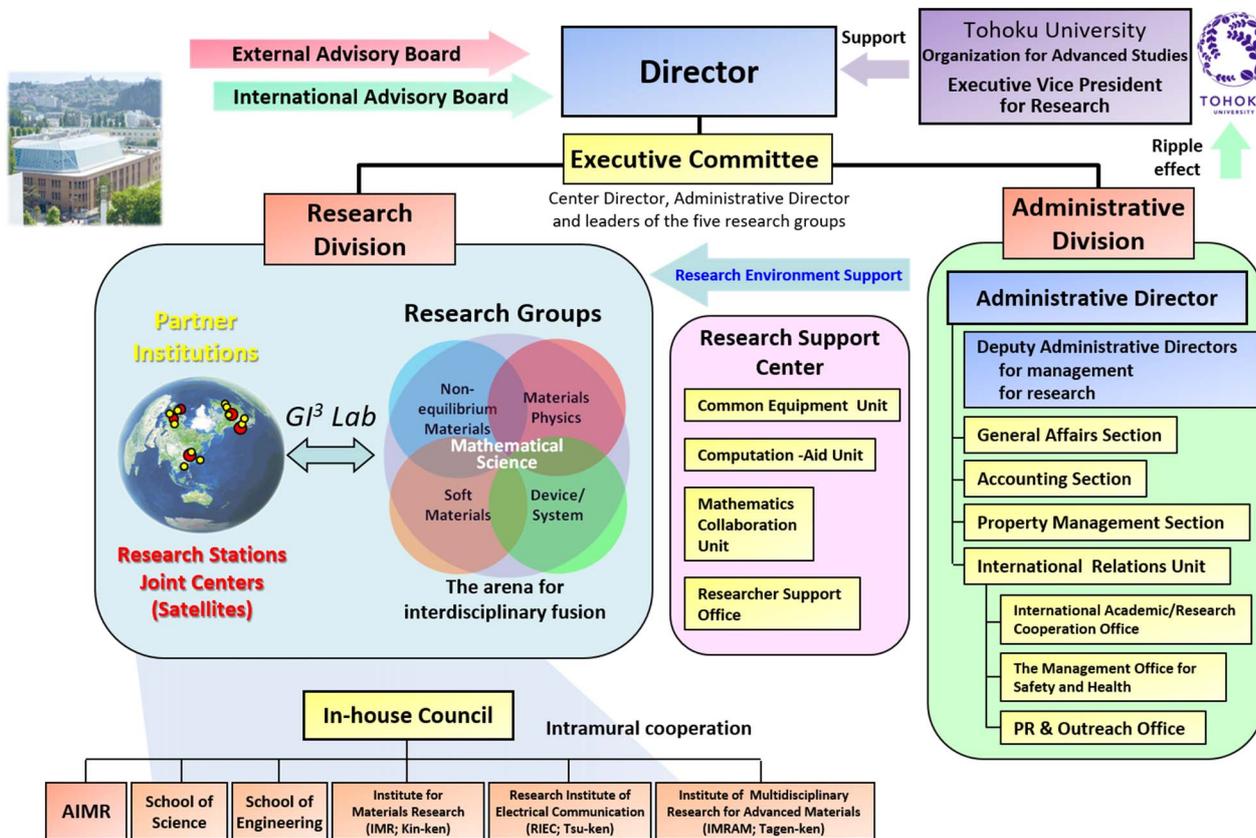
| Name | Age | Current affiliation (organization, department) | Academic degree and current specialties | Notes (Enter "new" or "ongoing") |
|---------------------------------------|-----|---|---|-------------------------------------|
| 1. Tadafumi Adschiri* | 59 | Tohoku University, Advanced Institute for Materials Research | Dr. of Engineering / Hybrid Materials, Supercritical Fluid Technology | ongoing |
| 2. Tomoteru Fukumura* | 47 | Tohoku University, Advanced Institute for Materials Research | Dr. of Engineering / Solid State Chemistry | new |
| 3. Ayumi Hirano* | 47 | Tohoku University, Advanced Institute for Materials Research | Dr. of Science / Bio-devices | new |
| 4. Yasuaki Hiraoka* | 39 | Tohoku University, Advanced Institute for Materials Research | Dr. of Science / Mathematics (Applied Topology and Dynamical Systems) | ongoing |
| 5. Motoko Kotani* | 57 | Tohoku University, Advanced Institute for Materials Research | Dr. of Science / Mathematics (Geometry) | ongoing |
| 6. Dmitri Valentinovich Louzguine* | 49 | Tohoku University, Advanced Institute for Materials Research | Dr. of Engineering / Materials Science | ongoing |
| 7. Shigemi Mizukami* | 44 | Tohoku University, Advanced Institute for Materials Research | Dr. of Engineering / Applied Physics, Spintronics | ongoing |
| 8. Hideo Ohno* | 62 | Tohoku University, Research Institute of Electrical Communication | Dr. of Engineering / Nanoelectronics | ongoing |
| 9. Shin-ichi Orimo* | 51 | Tohoku University, Advanced Institute for Materials Research | Ph.D. / Materials Engineering and Chemistry | ongoing |
| 10. Kosmas Prassides | 59 | Tohoku University, Advanced Institute for Materials Research | D. Phil. / Chemistry, Molecular | ongoing |

| | | | | |
|----------------------------|----|--|---|---------|
| | | | Materials | |
| 11. Eiji Saitoh* | 45 | Tohoku University, Advanced Institute for Materials Research | Dr. of Engineering / Quantum Nano Science | ongoing |
| 12. Seiji Samukawa* | 58 | Tohoku University, Institute for Fluid Science | Dr. of Engineering / Nano-Process Engineering | ongoing |
| 13. Hiroshi Suito | 55 | Tohoku University, Advanced Institute for Materials Research | Dr. of Engineering / Mathematical Modeling and Numerical Simulation | new |
| 14. Takashi Takahashi* | 65 | Tohoku University, Advanced Institute for Materials Research | Dr. of Science / Solid-State Physics | ongoing |
| 15. Katsumi Tanigaki* | 62 | Tohoku University, Advanced Institute for Materials Research | Dr. of Engineering / Nano Materials Science | ongoing |
| 16. Masahiro Yamashita* | 62 | Tohoku University, Advanced Institute for Materials Research | Dr. of Science / Coordination Chemistry | new |
| 17. Yuichi Ikuhara* | 58 | The University of Tokyo, School of Engineering, Institute of Engineering Innovation | Dr. of Engineering / Ceramics, Electron microscopy | ongoing |
| 18. Mingwei Chen* | 51 | Johns Hopkins University, Whiting School of Engineering | Dr. of Engineering / Materials Science | ongoing |
| 19. Yong P. Chen | 37 | Purdue University, School of Electrical and Computer Engineering | Ph.D. / Condensed Matter Physics, Nanotechnology | new |
| 20. Tomasz Dietl* | 66 | Polish Academy of Sciences, Institute of Physics | Ph.D. / Condensed Matter Physics (Theory) | ongoing |

| | | | | |
|-------------------------|----|--|--|---------|
| 21. Alan Lindsay Greer* | 61 | University of Cambridge, Department of Materials Science & Metallurgy | Ph.D. / Metallurgy & Materials Science | ongoing |
| 22. Ali Khademhosseini* | 41 | Harvard-MIT Division of Health Sciences and Technology, Brigham and Women's Hospital, Harvard Medical School | Ph.D. / Bioanalysis, Microfluidics & Biomaterials | ongoing |
| 23. Chris Pickard* | 43 | University of Cambridge, Department of Materials Science & Metallurgy | Ph.D. / Computational Materials Science Theoretical Condensed Matter Physics | new |
| 24. Thomas P. Russell* | 64 | University of Massachusetts, Polymer Science and Engineering Department | Ph.D. / Polymer Science and Engineering | ongoing |
| 25. Alexander Shluger* | 62 | University College London, Department of Physics and Astronomy | Ph.D. / Computational Materials Science, Condensed Matter Physics (Theory) | ongoing |
| 26. Winfried Teizer* | 46 | Texas A&M University, Department of Physics and Director of Center for Nanoscale Science and Technology | Ph.D. / Nano-Physics | ongoing |
| 27. Li-Jun Wan* | 59 | University of Science and Technology of China | Ph.D. / SPM, Electrochemistry, Nanomaterials | ongoing |
| 28. Qi kun Xue* | 53 | Tsinghua University, Department of Physics | Ph.D. / Surface Science | ongoing |

World Premier International Research Center Initiative (WPI) Appendix 2. Diagram of Center Management System

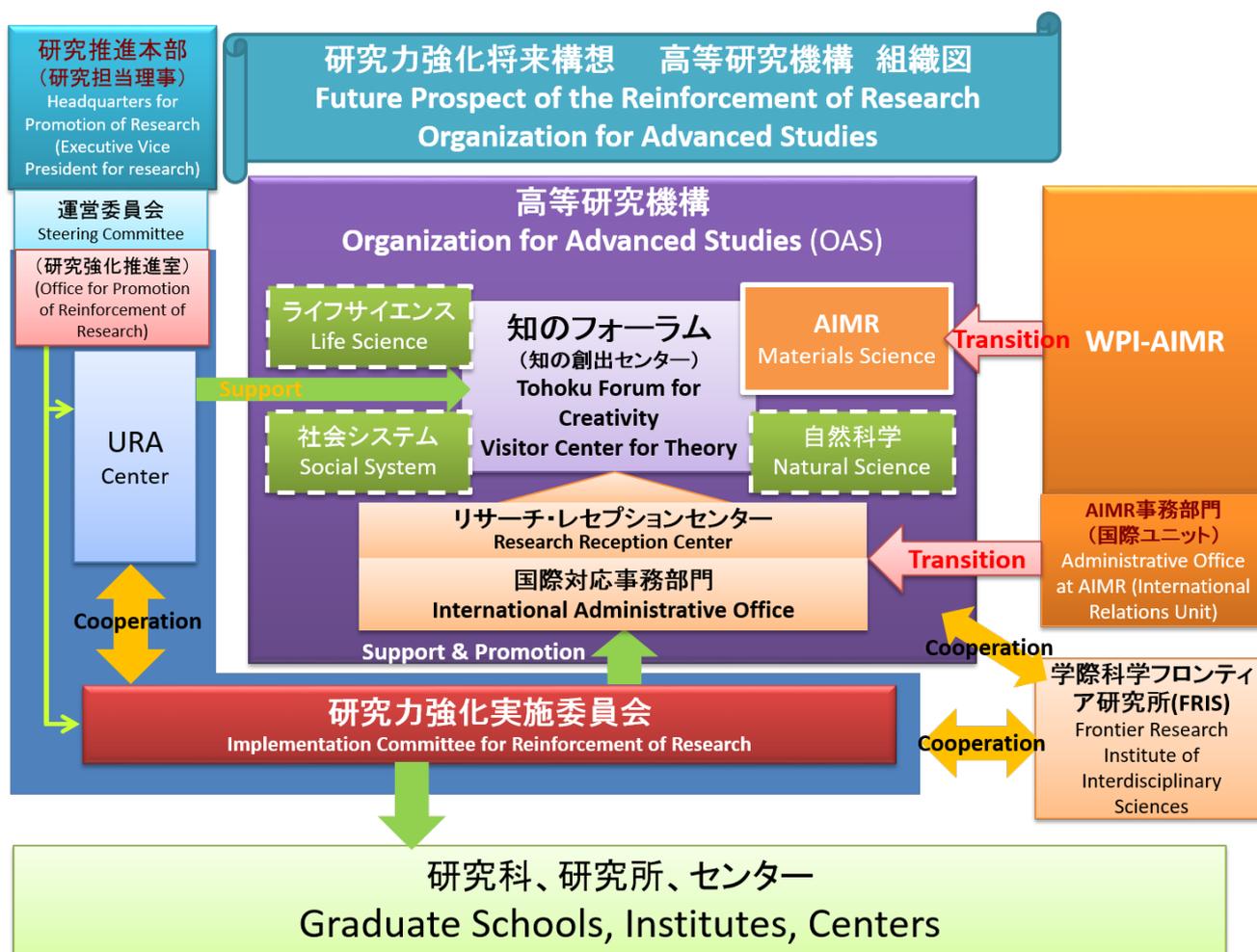
Organization at AIMR



World Premier International Research Center Initiative (WPI)

Appendix 3. Position of the Center within Host Institution

* Diagram the Center's position within the organization of the host institution, and describe that positioning using excerpts from the institution's mid- to long-term plan. If the plan has not been established yet, describe the consideration being given to the Center's positioning.



In the “**Third Mid-term Plan**” (from April 1st, 2016 to March 31st, 2022) of Tohoku University, the followings are stated (extract of the part relating to AIMR):

Article 2 Measures for achieving research goals

(2) Measures for achieving goals related to the system and environment for implementing research

②-1 Establishing institutes pursuing world-leading research

“In order to implement the cutting-edge research with all strength of this university, we steadily propel the reinforcement of the materials research field (**Advanced Institute for Materials Research**) firstly placed in Organization of Advanced Studies. In addition, we put other fields or research organizations in the Organization of Advanced Studies and construct world-leading research environment and research support system. To achieving the goal, we also promote the organic cooperation among Organization of Advanced Studies, graduate schools and research institutes.”

World Premier International Research Center Initiative (WPI)

Appendix 4. Resource Allocation Plan for Sustaining and Advancing the WPI Center

| Annual Plans (FY 2017 – FY 2021) | | | | | |
|---|--|---------------|---------------|---------------|---------------|
| <Fund > | | | | | |
| (million Yen) | | | | | |
| Fiscal Year | 2017 | 2018 | 2019 | 2020 | 2021 |
| - WPI grant | -(*) | -(*) | -(*) | -(*) | -(*) |
| - Funding from host institution | 763.5-863.5 | 763.5-863.5 | 763.5-863.5 | 763.5-863.5 | 763.5-863.5 |
| (details) | | | | | |
| Personnel | 628.7 | 628.7 | 628.7 | 628.7 | 628.7 |
| Project activities | 192.8 | 192.8 | 192.8 | 192.8 | 192.8 |
| Travel | 20.0 | 20.0 | 20.0 | 20.0 | 20.0 |
| Equipment | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Other research projects | 17.0 | 17.0 | 17.0 | 17.0 | 17.0 |
| Costs of Satellites | 5.0 | 5.0 | 5.0 | 5.0 | 5.0 |
| - Funding from external sources | 2200.0 | 2200.0 | 2200.0 | 2200.0 | 2200.0 |
| Total | 2963.5-3063.5 | 2963.5-3063.5 | 2963.5-3063.5 | 2963.5-3063.5 | 2963.5-3063.5 |
| | depending on the amount of the incentive allocated | | | | |
| <Personnel> | | | | | |
| (person) | | | | | |
| Fiscal Year | 2017 | 2018 | 2019 | 2020 | 2021 |
| - Personnel resources from host institution | 124 | 124 | 124 | 124 | 124 |
| - Faculty members (including researchers) | 36 | 36 | 36 | 36 | 36 |
| Full-time | 26 | 26 | 26 | 26 | 26 |
| Concurrent | 10 | 10 | 10 | 10 | 10 |
| - Postdocs | 48 | 48 | 48 | 48 | 48 |
| - RA etc. | 17 | 17 | 17 | 17 | 17 |
| - Research support staffs | 5 | 5 | 5 | 5 | 5 |
| - Administrative staffs | 18 | 18 | 18 | 18 | 18 |

(*) Do not include expected grant.

- When entering amounts, round down numbers to the first decimal.

- When funding is stated in a range between two amounts, explain the reason for the lower and upper amounts and fluctuations between them.

< Measures to be implemented from FY 2017 >

- Strategy and action plan for allocating personnel (posts) , space, and others measures required for the Centers' Progress.

The Center will formulate an action plan along the organizational conception of personnel and financial resources based on the dialogs and consultation with the host institution (President, Executive Vice President in charge and the heads of the related departments) and materialize the plan. In particular, AIMR is the first institute affiliated to Organization for Advanced Studies (OAS) established by the Tohoku University's Global Initiative and Tohoku University will provide maximum support for maintaining AIMR's permanence and independency.

Strategy and action plan for securing the appropriate number of members

Based on the term limit system of faculties which utilize the resources (ten tenure positions and funds) provided by the host institution, the Center will tackle the establishment of tenure-track system in cooperation with the host institution and the related departments.

Action plan for obtaining appropriate space

The host institution will continue to provide AIMR with the floor area about 17,300 m², land, buildings, facilities and infrastructure which have been prepared for AIMR during the period of the WPI program.

Strategy and action plan for carry out other necessary measures

- Measures for preparing the research facilities

The host institution will provide support for the increase of the use of common equipment and the establishment of the system for collecting charge in order to secure the financial resources to manage the Common Equipment Center stably.

- Measures for supporting young researchers and researchers from abroad

By utilizing the resources provided by the host institution and the resources independently acquired by the Center, support for young researchers will be continued by employing them as postdoctoral researchers (PDs) or research assistants (RAs). As well, travelling overseas by young researchers will continuously be supported through the Research Support Center placed at the OAS.

- Measures for maintaining the functions of overseas satellites

By utilizing the resources provided by the host institution, the Center will continue to exchange researchers and hold joint workshops with the overseas satellites (University of Cambridge, the University of Chicago, Chinese Academy of Sciences, University of California, Santa Barbara, and Fraunhofer ENAS) and other partner institutions and maintain the international partnership.