

Application for Academy Center Certification World Premier International Research Center Initiative (WPI)

Host Institution	Tohoku University
Research Center	Advanced Institute for Materials Research (AIMR)
Host Institution Head	Susumu Satomi (Apr. 2012 - Mar. 2018), Hideo Ohno (Apr. 2018 -)
Center Director	Motoko Kotani (Apr. 2012 - Sep. 2019), Shin-ichi Orimo (Oct. 2019 -)
Administrative Director	Masaru Tsukada (Apr. 2012 - Mar. 2018), Susumu Ikeda (Apr. 2018 -)

Please prepare this application based on the content of your center's progress report and the progress plan you submitted for the center's final evaluation. Summarize the center's future plans with regard to the following 6 items within three A-4 pages. (Also fill out the appendices at the end of this form.)

1. Overall Image of Your Center

* Describe the Center's overall image including its current identity.

The mission of AIMR is to create new materials with innovative functions through an ingenious method of atomic and molecular control departing from traditional approaches, construct devices based on new fundamental paradigms, and contribute to society by building a foundation for safe and rich life. In order to achieve this mission, AIMR stipulated its identity as "discovering common elements and universal principles among different material fields and creating new materials science which can predict new functions," and proposed a new research strategy, "**mathematics-materials science collaboration.**" Under the leadership of Prof. Motoko Kotani, a mathematician, AIMR strongly promoted mathematics-materials science collaboration unprecedentedly at an institutional level. In particular, at the initial stage of this challenge, AIMR organized a system for the mathematics-materials science collaboration by establishing Mathematics Unit and Interface Unit (these two units have been unified into Mathematical Science Group), and setting three Target Projects. Based on such highly motivated measures, AIMR has published high quality papers appearing in *Science*, *Nature's sister journals*, *Physical Review Letters* and so on. AIMR also focused on strengthening international cooperation network with world-leading institutions, and now AIMR is recognized as a hub of international collaborations and global brain circulation.

Although the English name of the center, Advanced Institute for Materials Research (AIMR), will be never changed, Japanese name of AIMR was modified on April 1st, 2017 in order to make the name more consistent with the present AIMR's status and fit the university's organization.

In October 2019, AIMR plans to install Prof. Shin-ichi Orimo (current AIMR Deputy Director, Principal Investigator, and the group leader of Device/System Group), as the new Center Director. Prof. Orimo, a specialist of materials development and device fabrication, has participated in the AIMR's mathematics-materials science collaboration (Target Projects) in the past several years and has the potential ability to achieve the ultimate goal of AIMR, creation of new materials and devices which can contribute to society

based on the new scientific principles established by the mathematics-materials science collaboration at AIMR. Under the leadership of the new center director, AIMR will raise the mathematics-materials science collaboration to the next stage where we develop real materials which contribute to society.

2. Research Activities

* Describe how the center will challenge new research fields and adopt new strategies.

Through newly launched Advanced Target Projects, AIMR will deepen and mature the mathematics-materials science collaboration that has been developed over the past half a decade, and make 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,”** and AIMR is recognizing that these will be future priority areas. In the area **1)**, in order to create new device technologies based on recent spin physics, we will facilitate a new theoretical principle to control energy and information transfer with mathematical guidance and will develop various energy saving devices and a new power generation system. Furthermore, we will focus on not only spin but also light elements (such as hydrogen) and biomolecules as important elements to produce functions of materials and try to create real materials which will contribute to society. In the area **2)**, AIMR implemented target projects 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 guiding principles to find new structures, and to realize the proposed structures. We also 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.

Another recent global trend is **“application of big data analysis by high performance computing.”** 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. Along these lines, AIMR has already produced some promising results, 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. Based on these measures, AIMR plans flexible and quick strategy in line with present needs, and will contribute to society by creating revolutionary functional materials based on the new materials science born at AIMR.

3. System for Managing the Research Organization

* Describe the research organization and management system that the center will use to carry out the research strategy and plan described above.

* In Appendix 1-3, list the Principle Investigators, enter the number of center personnel, and provide a diagram of the center's management system.

Center Directors Motoko Kotani (Apr. 2012 - Sep. 2019) and Shin-ichi Orimo (Oct. 2019 -) and PIs listed in **Appendix 1** will be united, pursuing pioneering research. In the past few years, eight new PIs (Professors), Tomoteru Fukumura, Yong P. Chen, Masahiro Yamashita, Ayumi Hirano, Hiroshi Suito, Chris Pickard, Takafumi Sato and Hayato Chiba joined AIMR and twelve PIs left AIMR. Although the change of the total number of PIs is not so large, the research areas to focus on have been slightly changed depending on the recent global trend of materials science. As shown in **Appendix 3**, 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, a global standard research environment and support system, the merit-based salary system, as well as the position of Administrative Director (a researcher hold this position) 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, if we can get support by WPI Academy, AIMR will maintain some of the joint laboratories established at overseas satellites (see the next **section 4**) and promote international collaboration through employing postdoctoral researchers at the joint laboratories and closely exchanging information.

Overall organizational structure of AIMR consists of 80 researchers (42 full-time members, 15 concurrent members and 23 postdocs; excluding research assistants), 28 research support staffs and 18 administrative staffs (see **Appendix 2**).

4. International Circulation of Best Brains

* Describe your policy and concrete plan for promoting the international circulation of the world's best brains, which is an important function of the WPI Academy.

Until FY2016, the proportion of researchers from abroad has been kept at around 50%. 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, in which 14 are overseas institutions. In particular, AIMR will continue to promote international collaboration by maintaining Joint Research Centers (joint laboratories) at three satellites, the University of Cambridge, the University of Chicago, and Tsinghua University which have been set up so far. At the Joint Research Centers, postdoctoral researchers employed by AIMR accelerated international joint research, and these efforts gave actual results in global brain circulation. The International Relations Unit (current International Affairs Center (IAC)) of the Administrative Division (current Research Support Division) contributed 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.

AIMR will maintain these international activities without any break, keep the position in the international materials research community, and materialize global brain circulation through implementing the following activities:

(1) Joint Research Centers: AIMR maintains and develops the above Joint Research Centers without any break and continues activities as a hub of international cooperation. We will reconsider research themes and researchers at the centers any time and stimulate the new evolution of research.

(2) Foreign PIs, international collaboration and exchange: AIMR continues to invite excellent researchers as PIs from overseas and performs fruitful collaborations through intensive discussion at AIMR. We will invite/dispatch young researchers from/to overseas partner institutions at any time when needed in order to activate global brain circulations of young generation. We hope that, using the budget of WPI Academy, we can continue GI³ Laboratory Program implemented during the WPI support period.

(3) Holding workshops with partner institutions: AIMR strengthens global network with existing 15 partner institutions, from present one-to-one style to many-to-many style, and AIMR acts as a hub in the global materials research community. We need to organize workshops with the partner institutions and expand the collaboration network to achieve the goal.

(4) Holding International Symposium: Every year, AIMR has organized AIMR International Symposium (AMIS) to provide a forum of academic exchange; invited prominent researchers including Nobel laureates, overlooked the forefront of wide range of materials science, and transmitted AIMR's research achievements to the world. Together with other three WPI centers related to materials science (MANA, iCeMS, and I²CNER), AIMR has jointly organized WPI one-day Symposium, for example, at the meetings of European Materials Research Society (E-MRS). Such efforts received a high evaluation and contributed to increasing the international visibility of WPI and WPI centers. We hope that we can continue such successful performances to establish the "WPI-brand" and contribute to the global brain circulation.

5. Support by Host institution

* Describe measures that the host institution will take to support and sustain your WPI center. Describe your strategy for extending the system reforms achieved by the center via the WPI program to the host institution and other institutions.

(1) Host institution's policy on support to sustain AIMR: The host institution, Tohoku University, continues to maintain the position of AIMR as a regular department of the university, providing AIMR with authority, resources and infrastructure given during the WPI period, even after the termination of the WPI program support. It can be seen in the statements of Tohoku University's "Third Mid-term plan" that strengthening AIMR and constructing world-leading research environment and research support system are among the university's goals. It is also expressed that Tohoku University will keep AIMR as the core to achieve the university's goals, "establishing world-leading research institutes" and "jumping to world class as the hub of global brain circulation" stipulated in SATOMI VISION (which is followed by Tohoku University Vision 2030 established by the current President Dr. Hideo Ohno), by putting AIMR in "Organization for Advanced Studies," the special ward for research. Tohoku University was named a Designated National University by the Japanese Government in June 2017 and the university has established world-leading research centers for four research fields (Core Research Cluster) including the research center for materials

science; AIMR is leading the materials science of Tohoku University as the core department of the world-leading research center for materials science.

(2) Expansion of the achievements of the system reform as a WPI center to the inside and outside of the university: The host institution, Tohoku University, established the “Organization for Advanced Studies (OAS),” the special ward for research comprised of WPI-type institutes, in order to spread the expertise of internationalization and system reform which AIMR cultivated as a WPI center over the whole university. Research system and administration system grown at AIMR have also spread into fields other than materials science, and Tohoku University is planning to establish new WPI-type institutes (other than materials science) under OAS. Tohoku University established International Affairs Center (developed from Research Reception Center of AIMR) and let this center organize “Tohoku University Day,” the meeting held at overseas institutions hosted by Tohoku University, run administrative affairs of international open laboratories such as “ELyTMaX (Lyon-Tohoku joint laboratory supported by CNRS, France)”, and Tohoku Forum for Creativity. These efforts are raising the value of administrative organizations of OAS and AIMR, and largely contributing to increasing international presence of Tohoku University.

6. Financial Measures

* In Appendix 4, describe the measures to be taken by the host institution for sustaining the center's functions and activities over a period of 5 years, and describe what external funding will be used to carry out the center's research activities.

President Satomi (Apr. 2012 - Mar. 2018) and President Ohno (Apr. 2018 -) pledged to keep permanent staff members (nine tenure faculties and ten administrative staff) already placed at AIMR, and add ten tenure positions. The five of the ten positions have been occupied by Professors Shigemi Mizukami (PI), Ayumi Hirano (PI), Hiroshi Suito (PI), Hayato Chiba (PI) and Associate Professor 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 the administrative/support staff members. Part of the resource will also be used to maintain cooperative relationship with the overseas satellites as mentioned above (see **Appendix 4**).

The host institution, Tohoku University, established the “Organization for Advanced Studies” to maintain and develop the excellent research and organizational system which AIMR cultivated in the past ten years, and fixed AIMR as a regular department of Tohoku University. These activities have been accepted as the relevant projects of the “National University Corporation Management Expenses Grants (to promote strengthening functions) 国立大学法人運営費交付金（機能強化促進分）” and “National University Corporation Grants for Promotion of Strengthening Functions 国立大学法人機能強化促進費” in FY2017 provided by the Japanese Government. AIMR will also make maximum efforts to keep positions for young experimental researchers (assistant professors and postdoctoral researchers) by external funds.

WPI Academy Center

Form 2 FY 2019 List of Principal Investigators

NOTE:

- Underline names of principal investigators who belong to an overseas research institution. Place an asterisk (*) by names of investigators considered to be ranked among world's top
- In case of researchers who newly participated in the center in FY 2019, state it in the "Notes" column.

<Results on October 1st, 2019>					Principal Investigators Total: 24	
Name	Affiliation (Position title, department, organization)	Academic degree specialty	Effort (%)*	Starting date of participation	Status of participation (Describe in concrete terms)	Notes
Center Director Shin-ichi Orimo*	Professor, AIMR, Tohoku University	Ph.D. / Materials Engineering and Chemistry	80%	From Jan. 2013	Usually stays at the center	newly appointed to Center Director
Deputy Center Director Hiroshi Suito*	Professor, AIMR, Tohoku University	Dr. of Engineering / Mathematical Modeling and Numerical Simulation	100%	From Apr. 2017	Usually stays at the center	newly appointed to Deputy Center Director
Tadafumi Adschiri*	Professor, AIMR, Tohoku University	Dr. of Engineering /Hybrid Materials, Supercritical Fluid Technology	80%	From start	Usually stays at the center	
Hayato Chiba*	Professor, AIMR, Tohoku University	Ph. D. /Informatics	100%	From Apr. 2019	Usually stays at the center	newly participated
Tomoteru Fukumura*	Professor, AIMR, Tohoku University	Dr. of Engineering/ Solid State Chemistry	80%	From Dec. 2016	Usually stays at the center	
Ayumi Hirano*	Professor, AIMR, Tohoku University	Dr. of Science / Bio-devices	80%	From Oct. 2016	Usually stays at the center	
Motoko Kotani*	Professor, AIMR, Tohoku University (Advisor to the Center Director)	Dr. of Science /Mathematics (Geometry)	20%	Director: From Apr. 2012 to Sept. 2019 Deputy Director: From May 2011 PI: From Mar. 2011	Usually stays at the center	stepped down from the position of Center Director newly appointed to Advisor to the Center Director
Dmitri Valentinovich Louzguine*	Professor, AIMR, Tohoku University	Dr. of Engineering / Materials Science	20%	Professor: From Dec. 2007 PI: From 2009	Cross-appointment (MathAM- OIL, AIST 80% and AIMR, Tohoku University 20%). Usually stays at the center	
Shigemi Mizukami*	Professor, AIMR, Tohoku University	Dr. of Engineering / Applied Physics, Spintronics	100%	From Nov. 2014	Usually stays at the center	
Seiji Samukawa*	Professor, Institute of Fluid Science, Tohoku University	Dr. of Engineering / Nano-Process Engineering	40%	From Apr. 2012	Usually stays at Institute of Fluid Science, close to the center, and participate in the center's activities	
Takafumi Sato*	Professor, AIMR, Tohoku University	Ph.D. /Physics	80%	From Apr. 2019	Usually stays at the center	newly participated

Katsumi Tanigaki*	Professor, AIMR, Tohoku University	Dr. of Engineering / Nano Materials Science	80%	From start	Usually stays at the center	
Masahiro Yamashita*	Professor, AIMR, Tohoku University	Dr. of Science / Coordination Chemistry	80%	From Dec. 2016	Usually stays at the center	
Yuichi Ikuhara*	Professor, School of Engineering, Institute of Engineering Innovation, The University of Tokyo	Dr. of Engineering / Ceramics, Electron microscopy	40%	From start	Stays at the center once a month	
Eiji Saitoh*	Professor, Department of Applied Physics, School of Engineering. The University of Tokyo	Dr. of Engineering / Quantum Nano Science	40%	From Apr. 2012	Stays at the center once a month	moved to the University of Tokyo (cross-appointment)
<u>Mingwei Chen*</u>	Professor, Johns Hopkins University, Whiting School of Engineering	Dr. of Engineering / Materials Science	20%	From start	•Stays at center four times (about two months in total) a year. •Attends the AIMR conference	
<u>Yong P. Chen*</u>	Professor, School of Electrical and Computer Engineering, Purdue University	Ph.D./ Condensed Matter Physics, Nanotechnology	20%	From Apr. 2017	•Stays at center three times (more than two months in total) a year. •Attends the AIMR conference	
<u>Tomasz Dietl*</u>	Professor, Head of Laboratory of Cryogenic and Spintronic Research, Institute of Physics, Polish Academy of Sciences	Ph.D./ Condensed Matter Physics (Theory)	20%	From Apr. 2012	•Stays at the center once a year •Attends the AIMR conference	
<u>Alan Lindsay Greer*</u>	Professor, Department of Materials Science & Metallurgy, University of Cambridge	Ph.D. in Metallurgy & Materials Science	20%	From start		
<u>Chris Pickard*</u>	Professor, Department of Materials Science & Metallurgy, University of Cambridge	Ph.D/Materials Theory	20%	From Apr. 2016	•Stays at the center once a year •Attends the AIMR conference •Conducts PD at AIMR Joint Research Center.	
<u>Thomas P. Russell*</u>	Professor, Department of Polymer Science and Technology, University of Massachusetts Amherst	Ph.D. in Nano-Science Technology	20%	From start	•Stays at the center once a year •Attends the AIMR conference	
<u>Alexander Shluger*</u>	Professor, Department of Physics and Astronomy, University College London	Ph.D. in Computational Materials Science, Condensed Matter Physics	20%	From start	•Stays at the center once a year •Attends the AIMR conference	
<u>Qi-kun Xue*</u>	Professor, Department of Physics, Tsinghua University	Ph.D. in Surface Science	20%	From start	•Dispatch a PD Researcher	

*Percentage of time that the principal Investigator will devote to his/her work for the center vis-à-vis his/her total working hours (total time for whole working activities including education, medical services, and others as well as research).

Researchers unable to participate in the center in FY 2019

Name	Affiliation (Position title, department, organization)	Starting date of participation
Yasuaki Hiraoka	Professor, Institute for Advanced Study, Kyoto University	From July 2016
Hideo Ohno	President, Tohoku University	From April 2012
Kosmas Prassides	Professor, Department of Materials Science, Graduate School of Engineering, Osaka Prefecture University.	From April 2013
Takashi Takahashi	Researcher, Sato Laboratory, AIMR, Tohoku University	From start
Ali Khademhosseini	Professor, California NanoSystems Institute, University of California Los Angeles	From November 2009
Winfried Teizer	Professor, NanoLab in the Physics Department, Texas A&M University	From November 2009

World Premier International Research Center Initiative (WPI) Diagram of management system

