REPORT OF THE 1ST ELEMENT STRATEGY INITIATIVE ADVISORY COUNCIL (ESIAC)

Chair: Hidetoshi Fukuyama
Reviewers: M. Coey, T. Miyazaki, H.-J. Freund, M. Tada, J.-M. Tarascon, T. Osaka, D. Ginley, M. Takigawa, P. Gumbsch, Y. Tomota
Advisers: M. Takata, T. Kanaya, S. Tsuneyuki

EXECUTIVE SUMMARY

The 1st meeting of the Element Strategy Initiative Advisory Council (ESIAC) was convened on 14 December, 2019 at TKP Garden City Premium, Yokohama Landmark Tower, 25F, following the open forum to introduce the activities of the Element Strategy Initiative (ESI) to the public on the preceding day.

We commend Program Director (PD) Kohei Tamao and the members of the core research centers for their ongoing efforts towards the progress of the Element Strategy Initiative Project (ESI-PJ).

The ESI-PJ was established by the Ministry of Education, Culture, Sports, Science and Technology, Japan (MEXT) in 2012 with the aim of "expanding the science of elements, which clarifies the functions and properties of materials, into a broad range of studies focusing on industrial applications in an effort to solve our resource problems".

In order to accomplish this not-easy task, MEXT formulated a project through the formation of four core research centers each with an individual focus, on magnets, catalysis/batteries, functional electronic materials, or structural materials. In each center, experts were selected across traditional research disciplines to form three groups, on material synthesis, measurement, and electronic theory/modeling. These groups were chosen to facilitate effective collaboration and pursue synergetic effects in close contact with industry. Collaborations with large-scale research infrastructure such as SPring-8/SACLA, J-PARC and super-computers were encouraged. Efforts to foster the next generation of scientists were encouraged, not only within each center but also among centers; this was expected to lead to the formation of a platform for materials science.

Hence the ESI-PJ is not merely a collection of individual research projects carried out by funding agencies, but a higher-level collaboration intended to reform research structure in Japan. MEXT's introduction of this particular vison into academic institutions has had great impact on both academia and industry, and allows scientific

seeds and social needs to meet more naturally than before, thus lowering the barriers between them. MEXT is to be applauded for this initiative.

The ESI-PJ is expected to act as a model to promote materials science research in the coming years in Japan. In this context it should be noted that, even though the ESI-PJ was triggered partly by the shortage of rare elements, the core concept of the project is to explore the possibilities of materials with green (abundant and non-toxic) elements and it is thus expected to play a key role in achieving the UN Sustainable Development Goals (SDGs).

ESIAC was asked to assess the research activities of the ESI-PJ over the past 8 years for a possible successful ending in 2022.

Program Director (PD) Tamao asked ESIAC for its opinions and recommendations on the research activities, management, and performance of the project, under the following terms of reference.

TERMS OF REFERENCE (TORs)

(1) Appropriateness of organizational structure and management
(2) Assessment of activities of each core center
(3) Comprehensive advice for the future of materials science in Japan from an international perspective

Observations and recommendations regarding TOR2 and those under TOR1 specific to each center are first summarized for each center in turn. Those under TOR3 and those under TOR1 that address the ESI-PJ as a whole are summarized at the end.

Observations and Recommendations

ESICMM: Satoshi Hirosawa

[TOR2] ***Assessment of activities of each core center***

The mission of ESICMM is 1) to establish a long-term research center on the basic materials science of permanent magnets and 2) to lay out the fundamental technologies and knowledge in this field and disseminate them among scientists in industry.

Specific goals are i) realization of ultimate permanent magnet materials, ii) realization of permanent magnet materials based on new Fe-rich compositions, iii) establishment of the basic science of permanent magnet materials, iv) dissemination and transfer of outputs into industry, noting that the basic ingredients for generating coercivity, the key feature of a permanent magnet, are internal energy barriers.

ESIAC recognizes that this center has responded very well to the original TORs. The research results are excellent and world-leading. They include:

1) Success with Dy-free magnets by grain-boundary engineering (infiltration) with a wise focus on the optimization of Nd-Fe-B. This focus was triggered by a

paradigm shift due to the discovery of ferromagnetism at the grain boundary by electron holography and XMCD. This is a great achievement of the Center.
2) Discovery of new 1-12-type compounds.
3) Progress on the very difficult problem of coercivity by combining micromagnetic simulation with atomic simulation of one grain.
4) Synergetic efforts to find a new processing route, grain boundary infiltration, and identification of new phases with theoretical contributions and a systematic thermodynamic database.
5) Success in communicating with the broader materials synthesis community at Tohoku Univ., Kyoto Univ. and NIMS.
6) Establishment of a vision for a core center for academia-industry cooperation on permanent magnets.

The following are the comments of ESIAC regarding further development of this Center.
1) In order to gain more insight into the grain boundary phases, accurate information in modeling and experiment will be needed.
2) Activities across centers are encouraged.
3) The Center should take note of recycling and develop a more integrated vision regarding sustainability/resources, including end of life-cycle assessment for new products.
4) More researchers may be needed to work on material synthesis.
5) The Center may need to think in future beyond materials synthesis and about the generalization of the process science.

[TOR1] ***Appropriateness of organizational structure and management***
ESIAC understands that the Center is well managed and integrated, and has very creative collaboration with SPring-8. It also has a good vision, with emphasis on science and creative contacts with industry, and this has led to the uptake of early results by industry.
ESIAC recommends that this Center collaborates with other centers for possible improvements to catalytic activities through the application of magnetic fields, and to apply grain-boundary engineering to interface design of alloy anodes in batteries.
ESIAC expects that this Center will contribute to the revitalization of the magnetic materials community in Japan.

For further development, ESIAC notes that:
1) There are too few patents and the Center lacks a patent strategy.
2) More exchange of investigators/students between institutions is encouraged.
3) Regarding recycling, the Center needs to talk to industry to develop a strategy, especially in the context of life-cycle analysis.
4) Collaboration/competition areas between academia/industry should mutually be made clear.
5) The collaboration between ESICMM and MagHEM (NEDO) projects should be made clearer.
6) Cultivation of the younger generation of human resources is necessary.

TIES: Hideo Hosono

[TOR2] ***Assessment of activities of each core center***

ESIAC congratulates this Center for the many substantial scientific achievements based on the vision of the leader, H. Hosono. These include: 1) overcoming traditional material design concepts rooted in past experience, 2) exploring the frontier in electronic materials by unconventional combinations of abundant and non-toxic elements, 3) establishing new design concepts and guidelines for further advancement of material technologies.

A well-defined roadmap for the comprehensive exploration of materials in the first 3 years (phase 1), was followed by materials selection in phase 2. Four focus areas were presented as phase 3, with a view to collaboration with industry. These are i) semiconductors, ii) high κ dielectrics/ferroelectrics, iii) hydrogen, and iv) collaboration between theory and synthesis together with rapid screening through materials informatics.

About 20 examples were introduced to ESIAC, which regarded the results overall as a brilliant set of materials with complex functionality, especially the 2d electrides, amorphous zinc silicate, hafnium oxide (not a perovskite, and stable at high temperature), achieved through daily collaborations (involving students) with nearby research institutes, NIMS and KEK-PF. However, ESIAC was disappointed with the progress in focusing on core concepts or the selection of particularly promising materials for industrial application. It noted that the Center has made little reference to the original TORs and obviously lacks focus.

ESIAC notes that the results are great basic science and provide very nice examples of uniting synthesis and many analytical techniques to solve a series of important problems. Hosono could be considered as a national treasure.

At the same time, ESIAC notes that Hosono's very strong leadership might be seen to have more benefit if the role and achievements of specific PIs had been more clearly presented.

[TOR1] ***Appropriateness of organizational structure and management***

The Center director demonstrates an inspiring scientific leadership. ESIAC would like to have seen cooperation between centers through, for example, ammonia synthesis.

In order to avoid overloading the leader, ESIAC suggests the appointment of a deputy (someone with experience in industry) and/or administrative support for outreach, intellectual property, and industrial contacts.

ESIAC appreciates that this Center is active in pursuing synergetic effects involving the younger generation including monthly meetings, a camp meeting, and international expansion through the JSPS Core-to-Core Program. It also has a clear plan to develop an Electronic Materials Institute after the ESI-PJ ends.

ESISM: Isao Tanaka

[TOR2] ***Assessment of activities of each core center***

ESIAC appreciates the courage of this Center in addressing the old but very difficult problem of overcoming the competition between ductility and strength. Instead of adding extra elements as is commonly done, the Center is trying to achieve this target by focusing on bulk nano-materials (BNM). On the basis of the discovery of enhanced ductility in systems consisting of nano-grains that cannot be understood by simple dislocation theory, the Center proposes a concept based on *plastons,* a collective motion of atoms. Through experiments on the size dependences of plastic deformation modes in Mg, a *plaston* diagram has been proposed, and the *plaston* concept has been extended to brittle materials.

ESIAC recognizes very remarkable progress with the development of nanostructured strong yet ductile steels, Mg-, and Ti-alloys. On the computational side, the software "phonopy" has quickly found widespread use and international recognition.

However, ESIAC considers the *plaston* concept to be ill defined, and not a worked-out theory/model. For example, the size and pattern of spatial deformations probably results from several competing known mechanisms that have not yet been clarified experimentally. On the theoretical side, ESIAC was confused by the explanation of the *plaston* nucleation process at grain boundaries based on first principles phonon calculations of ideal bulk crystals. The transition from *plaston* to known defects or deformation modes has not been worked out.

ESIAC has some concerns that the PD's recommendations reinforce the *plaston* concept because the Center was approved with *plaston* as a keyword. ESIAC encourages the Center to cope with the great challenge to exploit collective atomic motion in generating ductility in BNM. ESIAC recommends pursuing further work to identify and quantify the basic concepts demonstrated to date, especially making use of national facilities like SPring-8 and J-PARC, without relying on the linguistics of a *plaston* concept.

[TOR1] ***Appropriateness of organizational structure and management***

ESIAC did not understand why this Center had significantly fewer resources made available to it than the other centers. ESIAC recommends enhancing contacts/interactions with industry through internships, visits, and meetings (hosting industry researchers in their labs), and involving NIMS more in the Center.

ESICB: Tsunehiro Tanaka

[TOR2] ***Assessment of activities of each core center***

This Center is unique in having two research areas, catalysis and batteries. The aims of this Center are 1) development of high-performance catalysts with reduced use or without the use of critical elements, 2) development of rechargeable critical-element-

free high-performance batteries, 3) elucidation of guiding principles and description of the processes during catalysis and battery operation.

The Center has outstanding achievements. In catalysis, the development of non-PGM heterogeneous catalysts, Rh nano-films, and Mn-$YbFeO_3$ in a three-way-catalyst (TWC) are noteworthy. The planned activities in electrocatalysis are also noteworthy and should be encouraged. In batteries, the fact that the development of a Na battery and the first verification of its full-cell operation have been carried out by one of the PI's of this Center is noteworthy. The discovery of super-concentrated electrolytes is pioneering and innovative, and further development is expected once the international perspective has been properly incorporated.

ESIAC recommends the use of a variety of characterization tools (quantum beam, synchrotron, UV/VISs, IR, AFM, etc.) to strengthen the research activity on PGM-free catalysis.

[TOR1] ***Appropriateness of organizational structure and management***
This Center has unique opportunities with its two groups focusing on catalysis and batteries. These groups have quite different backgrounds, and there is no other similar example in the world. ESIAC applauds the interaction between the catalysis and battery parts of the Center.
Noting that they have commonalities in analysis, ESIAC notes that there is a good chance for the Center, especially the young researchers, to develop new ideas through interaction between the two parts of the Center, starting with collaborations between catalyst theory and battery theory. Collaboration with other centers, for example, collaboration with ESICMM for possible improvements to catalytic activities through the application of magnetic fields and for the application of grain-boundary engineering to interface design in batteries, and with TIES on catalytic materials, such as those for ammonia synthesis, would be creative.

PD: Kohei Tamao
[TOR1] ***Appropriateness of organizational structure and management***
[TOR3] ***Comprehensive advice for the future of materials science in Japan from an international perspective***
ESIAC thinks that the realization of the 10-year ESI-PJ with very talented scientists is excellent. The program is large enough to pick multiple important directions for Japanese industry.
In order to best achieve the project goals, however, there should be an overarching management structure. With more active overall management, synergetic effects could be realized in various stages, first within each Center and then among the four Centers, together with active collaborations with large-scale research facilities, synchrotron, quantum beams, and computational science. To unite the Centers, it is necessary to build bridges between them.

ESIAC encourages more cooperative actions to foster the younger generation and encourage female participation with an international perspective. In this context, a properly motivated central office could provide umbrella resources to the various projects, reducing administrative loads and serving as a nexus for communication and cross-fertilization.

More concretely,

1) ESIAC thinks that an international review like the present one should have been held much earlier, in view of the importance of the project and numbers of researchers involved.
2) ESIAC assumes that the present ESIAC report will be submitted not only to the PD, but also to all those in MEXT and the core centers who are involved in the ESI-PJ.
3) ESIAC thinks that it would be useful to have presented statistical information on the numbers of researchers, projects, publications, expenditure by category etc. for all centers in a uniform format.
4) Common metrics (not concepts but quantified metrics) are needed for all centers to put them all on the same playing field.
5) Key questions are:
   How is the budget allocated?
   What is the hiring policy? Is it systematic?
   What are the overarching goals for all Centers?
6) Money should be put aside to nucleate seed activities.
7) There is almost a complete absence of female PIs. A long-term strategy is needed. More frequent gatherings of all Centers with world experts and outstanding female speakers, and scholarship opportunities for women are encouraged.
8) ESIAC hopes to see greater participation in the project by scientists in private universities.
9) Without active overall management (communication is only one-way from management to the Centers), the Centers are almost autonomous.
10) A strong umbrella management/leadership is needed to bridge the four Centers, for example, by establishing co-shared PhD and post-doc programs and introducing a call for projects on “Anticipating Tomorrow’s Breakthroughs”. A yearly 2-day meeting of the whole ESI-PJ would be effective for enhancing synergetic effects.
11) Activities toward start-up companies should be encouraged.
12) The top management support system should be funded by MEXT.

ESIAC2019 Reviewers and Advisers

[Chairman]	
	Hidetoshi Fukuyama Adviser to the Chair and the President, Tokyo University of Science
[Reviewer]	
<Magnetic materials>	**Michael Coey** Professor, School of Physics and CRANN, Trinity College, Dublin
	Terunobu Miyazaki Professor, Tohoku University
<Electronic materials >	**David Ginley** Chief Scientist, The National Renewable Energy Laboratory, USA
	Masashi Takigawa Professor, The Institute for Solid State Physics, The University of Tokyo
< Catalysts >	**Hans-Joachim Freund** Director and Scientific Member, Fritz-Haber-Institute der Max Planck Gesellschaft, Germany
	Mizuki Tada Professor, Department of Chemistry, Graduate School of Science, Nagoya University
< Batteries >	**Jean-Marie Tarascon** Professor, Collège de France
	Tetsuya Osaka Professor, Department of Applied Chemistry, Faculty of Science and Engineering, Waseda University
<Structural materials>	**Peter Gumbsch** Director, Fraunhofer Institute for Mechanics of Materials IWM, Germany
	Yo Tomota Partnership Fellow, Visiting Researchers, The National Institute of Advanced Industrial Science and Technology (AIST)
[Adviser]	
<Synchrotron radiation >	**Masaki Takata** Professor, Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University
< Particle beam >	**Toshiji Kanaya** Professor, Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK)
<High performance computing>	**Shinji Tsuneyuki** Professor, Department of Physics, Graduate School of Science, The University of Tokyo

Element Strategy Initiative Advisory Council 2019
(ESIAC2019)

Day 1: Dec.13

[Open Session] Banquet Room A

15:30 - Registration desk open

16:00 - 16:05 **Opening remarks**
Hidetoshi FUKUYAMA (ESIAC Chairman)

16:05 - 16:15 **Expectations for Element Strategy Initiative**
Hiroki KUROSAWA (Director, Materials Science and Nanotechnology Development Division, Research Promotion Bureau, MEXT)
Shuichi SAKAMOTO (General Director, Cabinet Office)

16:15 - 16:25 **Introduction of the Element Strategy Initiative Research Project to Form Core Research Centers (ESI-PJ)**
Kohei TAMAO (Program Director)

16:25 - 17:15 **Activities of Core Research Centers** (10min/center)
The Elements Strategy Initiative Center for Magnetic Materials (ESICMM)
Satoshi HIROSAWA, Director General (NIMS)
Tokodai Institute for Element Strategy (TIES)
Hideo HOSONO, Representative (Tokyo Institute of Technology)
Elements Strategy Initiative for Catalysts and Batteries (ESICB)
Tsunehiro TANAKA, Director (Kyoto University)
Elements Strategy Initiative for Structural Materials (ESISM)
Isao TANAKA, Director (Kyoto University)

17:15 - 17:50 **Collaborative Research Facilities** (10min/each)
High Performance Computing Infrastructure (HPCI)
Shinji TSUNEYUKI (The University of Tokyo)
Particle beam facility
Toshiji KANAYA (High Energy Accelerator Research Organization (KEK))
Synchrotron radiation facility
Masaki TAKATA (Tohoku University)

[Get together Session]

17:50 - 18:00 **Banquet Room B (same floor)**
18:00 - 18:10 **Opening remarks**
18:10 - 20:00 **Exchange of opinions**
* Materials introduced in the session will be posted.

Element Strategy Initiative Advisory Council 2019
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Day 2: Dec.14

[Closed session] Banquet Room B

Participants: About 50
ESIAC2019 reviewers and advisors,
ESI-PJ related persons, government officials.

Chairman : Hidetoshi FUKUYAMA

8:30 - 8:40 Introduction (Hidetoshi FUKUYAMA)
8:40 - 8:55 Management system of ESI-PJ (Kohei TAMAO (Program Director))

< 1; The Elements Strategy Initiative Center for Magnetic Materials (ESICMM)>

9:00 - 9:30 Explanation of ESICMM Activities (Satoshi HIROSAWA)
9:30 - 9:50 Q&A
9:50 - 10:10 Closed discussions
10:10 - 10:20 Coffee Break

< 2; Tokodai Institute for Element Strategy (TIES)>

10:20 - 10:50 Explanation of TIES Activities (Hideo HOSONO)
10:50 - 11:10 Q&A
11:10 - 11:30 Closed discussions
11:30 - 12:30 Lunch Break

< 3; Elements Strategy Initiative for Structural Materials (ESISM)>

12:30 - 13:00 Explanation of ESISM Activities (Isao TANAKA)
13:00 - 13:20 Q&A
13:20 - 13:40 Closed discussions

< 4; Elements Strategy Initiative for Catalysts and Batteries (ESICB)>

13:45 - 14:15 Explanation of ESICB Activities (Tsunehiro TANAKA)
14:15 - 14:35 Q&A
14:35 - 14:55 Closed discussions
14:55 - 15:05 Coffee Break

< 5; Summary of ESI-PJ>

15:05 - 15:55 Closed discussions
15:55 - 16:15 Summary (Hidetoshi FUKUYAMA)
16:15 Closing (Kohei TAMAO)