Japan - EU Workshop on Substitution of Critical Raw Materials

– Final Report –

Scientific workshop to facilitate scientific matchmaking and to identify potential topics for future Japan – EU cooperative research

Tokyo, Japan
21-22 November 2011
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Introduction

The workshop convened researchers from the European Union and Japan to discuss the state-of-the-art in R&D related to the substitution of materials of concern due to demand-supply risks, toxicity or environmental impacts. This is a key concern as many technologies with significant socio-economic benefits face material requirements that are, or will be, negatively affected by demand-supply disruptions, or by concerns related to toxicity or negative environmental impacts. In particular, R&D activities are needed to improve our fundamental understanding of the development of new materials with a strongly reduced content of such materials or when possible eliminating their use completely.

In the course of the workshop, several research topics were identified and discussed for bilateral cooperation. The conclusions of this meeting will be provided to the European Commission and the Japan Science and Technology Agency (JST) for their input in the formulation of possible coordinated EU-Japan research activities in this field.

This expert consultation is in line with an ongoing international discussion to secure current and future access to critical materials.

The workshop was organised by the Japan Science and Technology Agency (JST), the EU Delegation to Japan, and the European Commission's Directorate General for Research and Innovation (DG RTD) and was held in Tokyo (Japan) on 21-22 November 2011.

The workshop was attended by 9 scientists from Denmark, Germany, Slovenia, Ireland, and Japan. The agenda is included as Annex 1 to this report and the list of participants is presented in Annex 2.
Scope and Objectives of the workshop

The topic of the workshop was the substitution of materials of concern due to demand-supply risks, toxicity or negative environmental impacts. Although other approaches exist, the substitution strategies remained limited to substituting a substance for another substance or substituting a new material for an old one. For a given application, the new material should at least provide the same performance, or offer compensating benefits.

This workshop was part of an ongoing discussion to secure current and future access to critical materials. It was the latest in a series of symposia, workshops and conferences of which the following can be considered as landmarks in promoting international cooperation on this subject:

- The "4th Joint Symposium on Elements Science and Technology Project/ Rare Metal Substitute Materials Development Project", organised by the Cabinet Office of the Japanese government, the Japanese Ministry of Education, Culture, Sports, Science and Technology (MEXT), and the Japanese Ministry of Economy, Trade and Industry (METI), Tokyo, 1 February 2010. European officials participated to the Program of the Symposium.

- The "Trans-Atlantic Workshop on Rare Earth Elements and Other Critical Materials for a Clean Energy Future", hosted by the US Department of Energy (DOE) and the Massachusetts Institute of Technology (MIT) in Cambridge, Massachusetts (US) on 3 December 2010, organized in cooperation with the European Commission, Directorate General for Research and Innovation DG RTD. European, Japanese and US officials and researchers participated in the meeting.

- The "Trilateral EU-Japan-U.S. Conference on Critical Materials for a Clean Energy Future" jointly organised by European Commission's Directorate General for Research and Innovation, the Japanese Ministry of Economy, Trade and Industry (METI), and the U.S. Department of Energy (DOE).

These events were crucial to exchange views and perspectives on the availability and supply challenges of critical materials. Emphasis has been on rare earth metals and other elements critical for clean energy generation and use. As such, a platform for cooperation has been established, which will facilitate cooperation in research between Europe, Japan and also the U.S.

The Tokyo workshop provided a bilateral technical forum for key European and Japanese experts with strong backgrounds in physics, chemistry and materials science and engineering to identify and discuss R&D opportunities for potential future coordinated research.

In particular, research avenues were explored that could improve our fundamental understanding on how to develop materials with a strongly reduced content of the materials of concern, or - when possible - eliminating their use completely.

This final report includes a number of potential research topics where synergy between the two regions can be beneficial and of mutual interest for EU and Japan research teams.
Methodology

Scientists from EU and Japan covered during their presentations a thorough overview of the most relevant topics related to the substitution of materials. One expert (Prof. Gutfleisch) participated to the meeting through a teleconference call. The list of the presentations is given in Table 1. The abstracts are included in Annex 3 of this report.

At the end of both scientific sessions and during the final report preparation session, open discussions were organised. During the course of the meeting and these discussions, examples were collected on three themes:

1. The development of materials by rational design, with focus on the interplay between theory and/or large-scale computational screening and experimental methods.
2. The synthesis or fabrication of nanostructures with enhanced functionality.
3. The use of advanced characterisation and measurement methods to determine how effects at the nano- or micrometer-level influence the materials' behaviour at the macroscopic level.

These themes were then illustrated with possible research topics which are included in the next section.

In several reports\(^1\), materials that have essential properties but are, or will be, negatively affected by demand-supply disruptions are considered to be "critical materials". The experts during this workshop paid indeed great attention to the opportunities to substitute such materials, and in particular to the rare earth (RE) metals\(^2\) (especially the heavy rare earths) and the platinum group metals (PGM)\(^3\).

However, the discussion went beyond these “traditional” critical materials. Several technologies were identified as potentially benefitting from the replacement of materials that currently might not considered to be scarce or critical but are of concern because of their toxicity or negative environmental effects.

\(^{1}\) A recent overview is given in the Resnick Institute Report on Critical Materials for Sustainable Energy Applications (August 2011).
\(^{2}\) RE metals: Y, Sc, and the lanthanides.
\(^{3}\) PGM: Pt, Pd, Ir, Rh, Ru, Os.
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<th>No.</th>
<th>Title of presentation</th>
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<td>Strategic materials relevant to permanent magnets and magnetic data recording</td>
<td>Michael Coey, Trinity College Dublin, IE</td>
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<td>Sadamichi Maekawa, Japan Atomic Energy Agency, Japan</td>
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<td>Role of Rare Metals in Material Technology and the Way to Substitute them</td>
<td>Komei Halada, National Institute for Materials Science, Japan</td>
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<td>9</td>
<td>Catalysis for sustainable energy: the challenge of harvesting and converting energy</td>
<td>Ib Chorkendorff, Technical University of Denmark, DK</td>
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**Outcome**

The experts proposed to foster potential R&D cooperation between EU and Japanese researchers to develop materials with a strongly reduced content of materials of concern, and where possible to exclude the use of these materials completely.

R&D activities could be developed along the lines of the three research themes.

1. Interplay between theory or large-scale computational screening and experimental methods for materials by rational design and intelligent interpolation.

   *Examples of topics*
   - Screening the family of Heusler alloys for uniaxial structures and/or high spin polarization
   - Screening catalysts for synthesis of fuels from sunlight.
   - Screening materials with appropriate band-gap and effective mass for solar energy harvesting

2. Synthesis/fabrication of nanostructures with enhanced functionality

   *Examples of topics*
   - Substitution of environmentally hazardous substances (e.g., Pb, Cd, Te, Hg, …)
   - Functional magnetic and spintronic materials
   - Narrow band gap semiconductors ($E_g < 2.2 \text{ eV}$)
   - Catalysts for hydrogen and oxygen conversion and evolution
   - Waste energy-harvesting materials/thermo-electrics

3. Advanced characterization and measurement methods to determine how effects at the level of the nano- or microstructure can influence macroscopic mechanisms

   Characterization methods should enable an understanding of electronic processes at the atomic level in relation to elemental substitution.

   *Examples of Topics*
   - Related software for advanced materials screening and evolutionary selection routines

The examples of topics are representative for cooperative R&D research but the list should not be considered as exhaustive.

The experts also made recommendations on what is needed successfully to implement R&D activities in this research domain:

- Materials research and the development of new materials in particular benefits from persistence, with long-term research programmes focusing resources on a time-scale needed to deliver materials solutions (10-15 years). Long-term persistence is needed to optimise the performance of materials. However, serendipity has often proven to generate unexpected results in materials research and flexibility in the research programmes is needed to follow up such opportunities.
A strong interplay between a broad theory approach, advanced modelling and focussed experimentation are essential to determine the most promising solutions from large numbers of possible materials combinations. Advanced characterisation equipment, including use of large-scale facilities may be indispensable.

There is a growing need in training researchers both in Japan and Europe. These researchers could be attracted to and benefit from international collaboration between Japanese teams and European consortia, in particular by promoting the exchange of researchers and in particular researchers in the early stages of their careers (PhD/postdoc level).

Opportunities for Japan – EU cooperation

The current economic, scientific, technological and industrial climate make topics related to the development of materials with a reduced content of materials of concern, timely and attractive for R&D funding. They create a promising application potential with clear societal benefits, in particular in the domains related to energy generation, transport or conversion. However, an improved fundamental understanding of the underlying physicochemical mechanisms of materials' substitution is urgently needed.

The suggested topics will strongly contribute to several EU policies, including the Critical Materials Initiative⁴, the Strategic Energy Technology Plan⁵, and the European Green Cars' Initiative Public Private Partnership.

The development of new materials with a reduced content of scarce metals is receiving substantial attention from the worldwide scientific community, especially in Japan and in Europe. Sufficient world-class expertise and infrastructures are available in Japan and in Europe to warrant coordinated research on a competitive basis. A proven record of already established collaborative efforts can be found in the scientific literature.

A sufficiently high and diversified number of topics has been identified for which further research at the level of the materials (rational materials design, synthesis, advanced characterisation …) is needed. This justifies the proposed joint research.

⁴ COM(2008) 699
⁵ COM(2009) 519
Conclusions

The workshop was an overall success, with expert scientists and representatives from funding agencies from both Japan and European countries integrated in the process. Presentations were of high quality and did stimulate intensive and fruitful discussions.

Topics have been identified as potential R&D topics to improve understanding of the basic science behind successful partial or complete substitution of materials that are critical for applications with significant socio-economic benefits on a global scale.

The experts strongly recommend the Japanese and European funding authorities to support coordinated research projects in the field of substitution of materials of concern due to demand-supply risks, toxicity or negative environmental impacts.

Contact for Information

Department of International Affairs
Japan Science and Technology Agency
jointeu@jst.go.jp
Tel. +81(0)3-5214-7375
Fax +81(0)3-5214-7379

EUROPEAN COMMISSION DIRECTORATE-GENERAL FOR RESEARCH AND INNOVATION
Directorate G – Industrial Technologies
Materials
erno.vandeweert@ec.europa.eu
Tel. (+32-2)29 95481
Fax (+32-2)29 60550
Annex 1

Japan-EU Workshop “Substitution of Critical Raw Materials”

Agenda

Date 21 - 22 November 2011
Venue 21 Nov, EU Delegation, 4-6-28 Minami - Azabu M1

22 Nov, 8F Conference Room, Tokyo Headquarters, Japan Science and Technology Agency

Organized by Japan Science and Technology Agency (JST), EU Delegation to Japan, and the European Commission Directorate-General for Research and Innovation (EC DG RTD)

Language English

Program

Day 1, November 21, 2011

13:00-13:30 Registration
13:30-13:45 Greeting Session
13:45-14:00 Introducing the Experts

Presentation by Japanese and EU experts - Day 1

Chair: Spomenka Kobe (Jozef Stefan Institute)

14:00-14:30 Overview of Japanese Research Activity on Critical Raw Materials ~Elemental Strategy Project~

Teruo Kishi, Advisor, National Institute for Materials Science

14:30-15:00 Strategic materials relevant to permanent magnets and magnetic data recording

Michael Coey, Professor, Trinity College Dublin

15:00-15:30 New functionalities in abundant element oxides: ubiquitous element strategy

Hideo Hosono, Professor, Tokyo Institute of Technology
15:30-16:00 Coffee Break

16:00-16:30 Magnetic materials in sustainable energy

*Oliver Gutfleisch* *via Skype (shared by Michael Coey), Professor, Leibniz Institute for Solid State and Materials Research*

16:30-17:00 Materials Design for Magnets -Focused on Magnetic Semiconductors-

*Sadamichi Maekawa*, Director, Japan Atomic Energy Agency

17:00-17:30 Discussion of the Day 1

17:45-19:30 Reception at EUROPA HOUSE - EU Delegation

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**Day 2, November 22, 2011**

*Presentation by Japanese and EU experts - Day 2*

**Chair: Hideo Hosono (Tokyo Institute of Technology)**

9:00-9:30 Rare Elements in Magnetic Materials

*Terunobu Miyazaki*, Professor, Tohoku University

9:30-10:00 Replacement and original magnet engineering options

*Spomenka Kobe*, Professor, Jozef Stefan Institute

10:00-10:30 Role of Rare Metals in Material Technology and the Way to Substitute them

*Kohmei Halada*, Group Leader, National Institute for Materials Science

10:30-11:00 Catalysis for sustainable energy: the challenge of harvesting and converting energy

*Ib Chorkendorff*, Professor, Technical University of Denmark

11:00-11:30 Discussion of the Day 2

11:30-12:30 Working Lunch

12:30-14:30 Report Preparation

14:30-15:00 Closing / Guidance
Annex 2

List of Participants

Japanese experts

Kohmei Halada
Research Center for Strategic Materials
National Institute for Materials Science (NIMS), Ibaraki, Japan

Hideo Hosono
Frontier Research Center & Materials and Structures Laboratory
Tokyo Institute of Technology, Yokahami, Japan

Teruo Kishi
National Institute for Materials Science (NIMS), Ibaraki, Japan

Sadamichi Maekawa
Advanced Science Research Center
Japan Atomic Energy Agency, Ibaraki, Japan

Terunobu Miyazaki
WPI Advanced Institute for Materials Research
Tohoku University, Sendai, Japan

European experts

Ib Chorkendorff
CINF, Department of Physics
Technical University of Denmark, Kgs. Lyngby, Denmark

Michael Coey
School of Physics/CRANN
Trinity College Dublin, Dublin, Ireland

Oliver Guttleisch
Institute for Metallic Materials
Leibniz Institute for Solid State and Materials Research Dresden (IFW Dresden), Dresden, Germany

Spomenka Kobe
Department for Nanostructured Materials
Jozef Stefan Institute, Ljubljana, Slovenia
Japanese officials

**Tu Geng**  
Department of International Affairs  
Japanese Science and Technology  
102-8666 Tokyo, Japan

**Hideo Nakajima**  
Department of International Affairs  
Japanese Science and Technology  
102-8666 Tokyo, Japan

**Takayuki Hasegawa**  
Department of International Affairs  
Japanese Science and Technology  
102-8666 Tokyo, Japan

**Daisuke Baba**  
Office for Materials Science and Nanotechnology Development  
Ministry of Education, Culture, Sports, Science and Technology, Japan  
100-8959 Tokyo, Japan

**Hotaka Homma**  
Office for Materials Science and Nanotechnology Development  
Ministry of Education, Culture, Sports, Science and Technology, Japan  
100-8959 Tokyo, Japan

**Saori Kanai**  
Office for Materials Science and Nanotechnology Development  
Ministry of Education, Culture, Sports, Science and Technology, Japan  
100-8959 Tokyo, Japan

EU officials

**Barbara Rhode**  
Science and Technology (S&T) Section  
Delegation of the European Union to Japan  
106-0047 Tokyo, Japan

**Akira Kimura**  
Science and Technology (S&T) Section  
Delegation of the European Union to Japan  
106-0047 Tokyo, Japan

**Erno Vandeweert**  
Industrial Technologies – Materials  
European Commission  
1049 Brussels, Belgium
Annex 3
Abstracts of the presentations (in order of presentation)

<table>
<thead>
<tr>
<th>Name</th>
<th>Teruo Kishi</th>
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<tr>
<td>Organization</td>
<td>National Institute for Materials Science</td>
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<td>Division/Department</td>
<td>Advisor</td>
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Presentation Title

Overview of Japanese Research Activity on Critical Raw Materials
~Elemental Strategy Project~

Abstract

It is little known that dominant items within the share of Japanese exports are not automobiles or computers, but primary products such as steels or magnets. We have been a world supplier of various and high-quality materials which have been produced by continuous innovation in the area of new functional structure designing as well as process engineering. As “critical elements” like rare-earths, which are gaining political attention, are taking important role in developing those advanced functional materials, Japan has been promoting national projects to tackle the current and coming situation. Some recent activities demonstrated by Ministry of Education, Culture, Sports, Science and Technology (MEXT) and Ministry of Economy, Trade and Industry (METI) will be introduced.
Name | JMD Coey  
---|---  
Organization | Trinity College Dublin  
Division/Department | School of Physics / CRANN  
Title | Professor  

**Presentation Title**

Strategic materials relevant to permanent magnets and magnetic data recording

**Abstract**

All high-performance permanent magnets are currently based on NdFeB or SmCo. Demand for these materials are currently running at about 80,000 tons per year and is set to increase with the advent of electric vehicles (about 3 kg per vehicle) and wind generators (about 700 kg per MW). Most critical are the heavy rare earth additives (Dy or Tb) required to provide the necessary temperature stability. It’s unlikely that these strategic elements, many of them coming from unregulated mines in South China can be entirely dispensed with. Furthermore, the prospects of a rare earth free high performance magnet are even dimmer for reasons that will be explained. Nevertheless, opportunities exist 1) to reduce heavy rare earth content by grain boundary engineering but also to develop rare earth free magnets with energy products intermediate between those of NdFeB and ferrite, where there is a significant market opportunity.

Concerning magnetic recording, although quantities in individual memories or hard disks are very small, of order 10 µg, the need for Pt or Pd in alloys with the necessary perpendicular anisotropy might be regarded as alarming. However, prospects of finding replacement alloys which do not use such scarce elements are good. Some examples will be presented.
Presentation Title

New functionalities in abundant element oxides: ubiquitous element strategy

Abstract

While most ceramics are composed of ubiquitous elements (the ten most abundant elements within the Earth’s crust), many advanced materials are based on rare elements. A ‘rare-element crisis’ is approaching owing to the imbalance between the limited supply of rare elements and the increasing demand. Therefore, we propose a ‘ubiquitous element strategy’ for materials research, which aims to apply abundant elements in a variety of innovative applications. Creation of innovative oxide materials and devices based on conventional ceramics is one specific challenge. This review describes the concept of ubiquitous element strategy and gives some highlights of our recent research on the synthesis of electronic, thermionic and structural materials using ubiquitous elements.
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<tr>
<th>Name</th>
<th>Oliver Gutfleisch</th>
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<tr>
<td>Organization</td>
<td>Leibniz Institute for Solid State and Materials Research Dresden (IFW Dresden), Dresden, Germany</td>
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<tr>
<td>Division/Department</td>
<td>Institute of Metallic Materials</td>
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<tr>
<td>Title</td>
<td>Professor</td>
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**Presentation Title**

Magnetic materials in sustainable energy

**Abstract**

A new energy paradigm, consisting of greater reliance on renewable energy sources and increased concern for energy efficiency in the total energy lifecycle, has accelerated research in energy-related technologies. Due to their ubiquity, magnetic materials play an important role in improving the efficiency and performance of devices in electric power generation, conversion and transportation.

Magnetic materials are essential components of energy applications (i.e. motors, generators, transformers, actuators, etc.) and improvements in magnetic materials will have significant impact in this area, on par with many “hot” energy materials efforts (e.g. hydrogen storage, batteries, thermoelectrics, etc.). Their increased implementation in these devices and related market growth of e.g. electric vehicles and wind turbines will depend critically on the price and stable availability of the rare earth metals.

State-of-the-art hard and soft magnets and magnetocaloric materials with an emphasis on their resource-efficient optimization for energy applications will be described. More specifically, the impact of hard magnets on electric motor and transportation technologies, of soft magnetic materials on electricity generation and conversion technologies, and of magnetocaloric materials for refrigeration technologies, will be discussed.

The synthesis, characterization, and property evaluation of the materials, with an emphasis on structure-property relationships, will be examined in the context of already existing and future bottle-necks in raw materials and in the supply chain.

Finally, options for recycling of rare-earth permanent magnets will be analyzed.

Presentation Title

Materials Design for Magnets — Focused on Magnetic Semiconductors —

Abstract

There is a growing interest in the computer simulation for improving properties and predicting novel functions in materials. This is because of the recent developments of supercomputing facilities and of numerical simulation techniques. Here, I focus on the materials design for dilute magnetic semiconductors [1] and discuss the recent progress.

Dilute magnetic semiconductors are particularly important because of possible spintronics device applications. Many magnetic oxides have been proposed to be room-temperature ferromagnetic semiconductors. However, most of the experimental data are still controversial and remain to be clarified. These materials are sometimes called UFO (unidentified ferromagnetic objects) with the similar situation to USO (unidentified superconducting objects).

In order to understand the nature of the correlations which develop between magnetic impurities in semiconductors and how they differ from that in a metallic host, we map the electronic state obtained by the band calculation based on density functional theory (LDA) onto the impurity Anderson model and perform the Quantum Monte Carlo (QMC) simulations on the model [2].

We have recently discovered a magnetic semiconductors, Li (Zn, Mn) As which may show both p-type and n-type properties. Various magnetic oxides and possible so-called $d^0$ ferromagnetism in non-magnetic oxides such as MgO with N impurities are proposed.

Abstract

Magnetic materials will be classified into spintronic materials, hard magnetic materials and soft magnetic materials. Especially, rare elements (noble metals and rare earth metals) are used in former two groups. Examples of these materials are summarized and some efforts to replace rare elements with others and/or to make rare elements free materials will be explained.

Spintronics materials

It is well known that both GMR (Giant Magnetoresistance) effect and TMR (Tunnel Magnetoresistance) effect contributed to the increase of recording density of DRAM and the realization of magnetoresistive memory MRAM. Especially, much interest is focused on high density MRAM in order to realize so-called Normally-off-Computer. The key technology is how develop a magnetic tunnel junction (MTJ) with high thermal stability and low energy consumption. In order to fabricate such MTJs, the importance of materials will be explained. We are searching noble-metal-free or rare earth-free junction materials. Our recent results will be introduced.

Hard magnetic materials

NdFeB permanent magnet is one of the important materials for recent advanced technological industry. In order to increase the thermal stability of the magnet property, a relatively large amount Nd is replaced by Dy. Due to the anti-parallel coupling of the magnetic moment of Dy with that of Fe, the energy product reduces. In addition, the natural supply of Dy is limited and it’s cost increases remarkably in recently. Dy-free or Dy-lean NdFeB magnets are strongly desired. Kato group (Yamagata University) is carrying out very attractive methods for this issues. I introduce their recent results. Finally, the various methods to replace rare elements will be summarized.
Abstract

Permanent magnets based on rare earths (REs), in particular the neodymium-iron-boron (Nd-Fe-B) type, have revolutionized the worlds of computing, motors/actuators and electrical/electronic devices. Furthermore, they are increasingly important in environmentally critical technologies like hybrid and pure electric vehicles (HEVs and EVs) as well as for wind turbines.

Suggestions will be given on how to drastically reduce or totally eliminate the need to use scarce and most expensive heavy rare earths (HREs) like terbium (Tb) and dysprosium (Dy, which are indispensable in high coercivity, high temperature applications and represent by far the highest expense in production of Nd-Fe-B magnets: neodymium (340$/kg), dysprosium (2950$/kg) and terbium (4300$/kg). All prices as of 4 Nov 2011 for RE metal 99% min.

A typical magnet for automotive or moderately high-temperature use employs about 30-24 weight percent Nd and 4–10 weight percent Dy or Tb, i.e., Dy/Nd = 0.2. Therefore the real problem in terms of critical supply lies in the heavy rare earths, rather than REs in general. It will be presented how these heavy rare earths can be reduced or even totally eliminated by advanced synthesis, characterization and modeling focused on grain boundary engineering, introducing modified grain boundaries and sophisticated control of the microstructure towards the nanoscale, as one of the possible solutions.

The other idea, which will be briefly presented and showed more in details by other experts is focused on new permanent magnets with no rare earth.

The new materials will be based on breakthrough ideas, innovative technologies and alternative materials rather than access to scarce or highly overpriced raw materials.
**Presentation Title**

Role of Rare Metals in Material Technology and the Way to Substitute them

**Abstract**

21st century is the century of innovation. Materials technology gives great contribute to innovation. Rare earth elements and rare metals have the possibility of novel functions which realize our dream on energy and environmental issue. In the presentation, Role of rare earth elements in NIMS research is presented as examples. The direction of the substitution of rare metals in to abundant metals is introduced. The fundamental approaches of reduce and alternative technology of rare earth elements and rare metals is also mentioned.
Catalysis for sustainable energy: The challenge of harvesting and converting energy

Abstract
For many decades to come we shall still rely on fossil resources and as new sustainable energy sources emerge there will be a need for averaging out the temporal variation. Both schemes will require extensive use of heterogeneous catalysts and the need for new electro- and photocatalysts will increase. In this presentation we will demonstrate a number of surface chemistry reactions, in which a combination of theoretical insight and interplay between experimental surface science on well-defined single crystal surfaces, model systems of nanoclusters deposited on planar surfaces, and measurements on supported catalysts have made identification of new catalyst possible [1]. Gaining fundamental insight allows for prediction power on what should be done in order to improve the catalytic activity and how we optimize their presence? Furthermore, we will also demonstrate that this principle can be extended to control selectivity and optimization of electrochemical reactions, for which we are exploring alternative catalyst for either reducing [2,3] or entirely replacing the scarce and expensive Platinum group catalysts [1,4].