

# 1<sup>st</sup> US-Japan Materials Genome Workshop

D a t e : June 23-24, 2015

V e n u e : International Congress Center "Epochal Tsukuba"  
2-20-3, Takezono, Tsukuba, Ibaraki, 305-0032, Japan  
<http://www.epochal.or.jp/eng/index.html>

Organization and planning: NIST, NIMS, and CHiMaD (Northwestern University)

Co-sponsors: JST, DOE, NSF

Cooperation: MEXT

## **Workshop rationale:**

Both the US and Japan are going to have new era of materials science research. It is the trial for new materials developments that promote fusions of database technology, high throughput materials syntheses technology and high throughput evaluation technology combined with computational sciences. It is recognized as "Materials Genome Initiative" in the US and this process starts to be applying for many materials developments.

Both countries have needs for large-scale infrastructure development in the coming decades, with expenditures estimated in the trillions of US dollars. To assist both countries in planning and designing less costly and more sustainable infrastructures, the development of advanced structural materials that will function in the required environments is needed.

By adopting the materials genome approach, it will help to design reliable materials based on predictive theoretical models and databases, thus reducing the time needed to develop these new materials. US and Japan have complementary strengths in these areas of research and development. By developing collaborations among researchers, accelerated progress will be made with more efficiency.

On the 14th U.S.-Japan Joint Working-Level Committee Meeting on Science and Technology Cooperation (JWLC; July 7, 2014), the importance of collaboration between US and Japan for the fusion of materials science, computational science and data technology and personal exchanges for this new research field was discussed. Then organizing the workshop for discussing

MG continuously was designated. This workshop is based on the discussion on JWLC. Calling upon a great amount of expertise in this field, this workshop is organized to accelerate the development of new materials research.

### **Themes:**

The workshop is designed to cover all aspects of the materials genome (MG) approach with particular emphasis on advanced structural materials for infrastructure utilization covering materials such as metal alloy, composites and ceramics. Topics include: materials by design, materials database creation, infrastructure needs for a MG focused on infrastructure materials. Invited lectures and parallel discussion sessions will be part of the two-day activity. The workshop will identify both important scientific and engineering challenges in these areas as well as avenues for collaboration.

Plenary talk which is consisted of the back ground and recent topics helps to understand the current circumstances of MG researches. In the group session, panelists provide topics as well as problems to be discussed. The discussions are summarized and shared in each group. Important challenging problems from the scientific points of view are also discussed and future collaborative research themes between both countries will be explored. After the workshop, policies and plans for the collaboration will be summarized as the report.

A workshop report will be compiled with special suggestions for collaboration and implementation.

## **DAY 1 June 23, 2015 (TUE)**

8 : 30 **Registration**

9 : 00 **Welcome and Opening Speeches** @Convention Hall 200

1. Sukekatsu Ushioda,  
National Institute for Materials Science (NIMS)
2. Yuko Nagano  
Ministry of Education, Culture, Sports, Science and Technology (MEXT)
3. Alexis C. Lewis National Science Foundation (NSF)
4. James Warren National Institute of Standard and Technology (NIST)

[Moderator: Yoshio Aoki (NIMS) and Robert Chang\* (Northwestern University)]

**Session 1** : 10 : 00-12 : 20 @Convention Hall 200

10 : 00-10 : 20

**Outline** : "Overview and Research Topics for the Materials Genome Workshop"  
Toyohiro Chikyow, NIMS

10 : 20-10 : 40

**Plenary Lecture 1** : "Overview of JST's Data-Driven Materials Research"  
Jun'ichi Sone, Japan Science and Technology Agency

10 : 40-11 : 30

**Plenary Lecture 2** : " The Materials Genome Initiative: NIST, Data, and Open Science"  
James Warren, NIST

11 : 30-11 : 50 Coffee Break

11 : 50-12 : 30

**Plenary Lecture 3** : "Overview of "Materials Research by Information Integration (MI<sup>2</sup>I)" Initiative"  
Kiyoyuki Terakura, NIMS

[Moderator: Toyohiro Chikyow\* (NIMS)]

12 : 30-12 : 40            Group Photo

12 : 40-13 : 30            Lunch

**Session 2 :** 13 : 30-14 : 20 @Convention Hall 200

**Special Lecture :** “Informatics Approaches in Materials Science “  
Isao Tanaka, Kyoto University

[Moderator: Taizo Sasaki\* (NIMS)]

14 : 20-14 : 40            Coffee Break

**Session 3 :** 14 : 40-16 : 30

General topics related to the MGI by Five parallel discussion groups

**Group 1a :** Materials design by calculation and modeling

@Conference Hall 201a

Short Lecturer

Koji Tsuda (University of Tokyo)

Vladan Stevanovic (Colorado School of Mines&NREL)

[Moderator: Taizo Sasaki (NIMS) & Wing Kam Liu\* (Northwestern Univ.)]

**Group 1b :** Materials design by simulation and modeling

@Conference Hall 201b

Short Lecturer

Tsuyoshi Miyazaki (NIMS)

Chioko Kaneta (FUJITSU Laboratories)

Jon Guyer (NIST)

Julia Medvedeva (Missouri Univ.S&T)

Alejandro Strachan (Purdue Univ.)

[Moderator: Naoto Umezawa\* (NIMS) & Monic Olvera (Northwestern Univ.)]

**Group 2 : Materials synthesis and data base**

@Conference Hall 202a

Short Lecturer

Toyohiro Chikyow (NIMS)

Atsushi Yamamoto (National Institute of Advanced Industrial Science  
and Technology, AIST)

Zach Trautt (NIST)

Sara Barron (NIST)

[Moderator: Takahiro Nagata (NIMS) & Darryl Butt\* (Boise State Univ.)]

**Group 3 : Materials characterization and data mining**

@Conference Hall 202b

Short Lecturer

Dam Hieu Chi (Japan Advanced Institute of Science and Technology,  
JAIST)

Yibin Xu (NIMS)

Martin Green (NIST)

Boris Wilthan (NIST)

[Moderator: Hideki Abe (NIMS) and Kevin Coakley\* (NIST)]

**Group 4 : Research Infrastructure for materials development**

@Conference Hall 406

Short Lecturer

Yasuo Koide (NIMS)

Shinji Kohara (NIMS)

Mike Bedzyk (Northwestern Univ.)

[Moderator: Hideki Yoshikawa (NIMS) & Cate Brinson\* (Northwestern Univ.)]

**Session 4 : 16 : 30-17 : 30 @Convention Hall 200**

Joint discussion with short reports from each group

[Moderator: Toyohiro Chikyow (NIMS) & Sara Barron\* (NIST)]

## **Day 2 June 24, 2015 (WED)**

**Session 5 :** 8 : 30- 10 : 30 @Convention Hall 200

MG for advanced structure materials

8 : 30- 9 : 10

**Plenary Lecture 4 :** “Materials Genomics: From CALPHAD to Flight”

Gregory Olson (Northwestern University)

9 : 10-9 : 50

**Plenary Lecture 5 :** “CVM as a theoretical tool in Integrated Computational Materials Designing”

Tetsuo Mohri (Tohoku University)

9 : 50-10 : 20

**Invited Talk :** “Introduction to Development of Materials Integration System in Structural Materials for Innovation Project, Cross-ministerial Strategic Innovation Promotion Program”

Masahiro Takemura (JST)

Yutaka Kagawa (University of Tokyo)

[Moderator: Koichi Tsuchiya (NIMS) & R.P.H. Chang\* (Northwestern Univ)]

10:20-10:40

Coffee Break

**Session 6 :** 10 : 40-12 : 40

MG for advanced structure materials

**Group 1a :** Materials design by calculation and modeling

@Conference Hall 201a

Short Lecturer

Ryoji Sahara (NIMS)

Mitsuhiro Itakura (Japan Atomic Energy Agency, JAEA)

Wing Kam Liu (Northwestern Univ)

[Moderator:Tomonori Kitashima (NIMS) & Francesca Tavazza\* (NIST)]

**Group 1b** : Materials design by simulation and modeling

@Conference Hall 201b

Short Lecturer

Jun Yanagimoto (University of Tokyo)

Zi-Kui Liu (Penn State Univ.)

Ed Garboczi (NIST)

Monica Olvera de la Cruz (Northwestern Univ.)

[Moderator: Takuya Kadohira (NIMS) &

Julia Medvedeva\* (Missouri Univ.S&T)]

**Group 2** : Materials synthesis and data base

@Conference Hall 202a

Short Lecturer

Ikuo Ohnuma (NIMS)

Junpei Sakurai (Nagoya University)

Darryl Butt (Boise State Univ.)

Srikanth Patala (North Carolina State University)

[Moderator: Masahiro Goto (NIMS) & Sara Barron\* (NIST)]

**Group 3** : Materials characterization and data mining

@Conference Hall 202b

Short Lecturer

Yoshitaka Adachi (Kagoshima University)

Kevin Coakley (NIST)

[Moderator: Yibin Xu (NIMS) & Martin Green\* (NIST)]

**Group 4** : Research Infrastructure for materials development

@Conference Hall 406

Short Lecturer

Yo Tomota (NIMS)

Cate Brinson (Northwestern Univ.)

Eswaran Subrahmanian (NIST)

[Moderator: Yoshiyuki Yamashita (NIMS) &

Mike Bedzyk\*(Northwestern Univ.)]

12 : 40-14 : 00            Lunch

**Session 7 : 14 : 00-17 : 20 @Convention Hall 200**

**US and Japan's Expectation to Materials Genome Initiative**

14:00—14:30

“DFT calculation over view of NIST”

Francesca Tavazza (NIST)

14:30—15:00

“Global Information Infrastructure”

Foster, Ian T, (University of Chicago)

15:00—15:30

“The Needs and Some Case Studies of Integrated Computational Materials Engineering in Boeing”

Donald S. Shih (Boeing Research & Technology)

15:30-16:00            Coffee Break

16:00—16:30

“Material and Process Designs in Toyota Central R&D Laboratories and Industry's Expectation for Materials Genome”

Masaya Kawasumi (Toyota Central R&D Labs)

16:30—17:00

“Alloy and Process Design and Development at General Electric: Using Computational Methods to Accelerate Technology Introduction”

Judson S. Marte (GE Global Research)

[Moderator: Yasuo Koide (NIMS) and James Warren\* (NIST)]



**Session 8 :** 17 : 00-17 : 30 @Convention Hall 200

Joint session: reports from groups; discussion; and future plans

[Moderator: Koichi Tsuchiya\* (NIMS) & R.P.H. Chang (Northwestern Univ)]

17 : 30 **Closing Remark**

Takahiro Fujita (NIMS)

@Convention Hall 200

18 : 00 **Banquet**

@ Multi-Purpose Hall