

## 10<sup>th</sup> International Workshop on Combinatorial Materials Science and Technology (COMBI2018)

## October 3-5 2018 Hotel Mielparque Yokohama, Yokohama, Kanagawa, Japan

http://tus-fujimotolab.jp/meeting/combi2018

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**Exhibitors** 

Comet Inc. https://www.comet-nht.com/company-e.html





## Crystals for a brighter future

SHINKOSHA CO., LTD. http://www.shinkosha.com/english/index.html **Sponsors** 



ACS Combinatorial Science https://pubs.acs.org/journal/acsccc



Rigaku Corporation https://www.rigaku.com/en

## **Foundation grants**

Kato foundation for Promotion of Science

公益財団法人 加滕科学振興会 Kate Foundation for Promotion of Science

## The Murata Science Foundation

公益財団法人 村田学術振興財団

SUZUKI FOUNDATION

Foundation Advanced Technology Institute

公益财团法人新世代研究所 FOUNDATION ADVANCED TECHNOLOGY INSTITUTE

## Preface

On behalf of the organizing committee of the 10<sup>th</sup> International Workshop on Combinatorial Materials Science and Technology, we welcome all of you to this Workshop.

It has passed 20 years since the combinatorial synthesis was focused as an innovative tool for new materials discovery. To encourage the combinatorial materials science and related technologies, we organized the first Japan-US Workshop on Combinatorial Materials Science and Technology at Maui in Hawaii in 2000. The Workshop was successful to provide cutting edge results obtained by combinatorial methodology or to share the knowledge for the combinatorial synthesis. At the same time, this workshop became a trigger to start some collaboration in different Institutions.

From 2006, this workshop became the International Workshop because European new members joined this Workshop. In 2010, we had attendees from Australia and this workshop became a major conference where the combinatorial methodology was discussed and the practical application of this method to various materials research could be seen.

In 2011, the Materials Genome Initiative started in the United States and this initiative gave impact to this Workshop. The 8<sup>th</sup> international Workshop was held in Australia and there we invited some researchers who were working on vertical materials screening with their own original database driven by automatic calculation.

This year, we celebrate anniversary for this 10<sup>th</sup> International Workshop on Combinatorial Materials Science and Technology in Yokohama, Japan. This time, we witness the research trend change in materials informatics because the fusion of vertical materials screening and high thought experimentation including combinatorial synthesis is inevitable to new materials discovery. Machine learning or deep learning was popular. However, still the data for screening is insufficient. To compensate the lack of data, some mathematical tools are necessary. In this workshop we invite speakers from various field and new topics are proposed.

I hope all of the attendees enjoy this Workshop and help you to understand the new trend in materials informatics.

Tayli Chiy

**Toyohiro Chikyow** 

The Chair of Organizing Committee, the the 10<sup>th</sup> International Workshop on Combinatorial Materials Science and Technology

## **Organizing committee**

GENERAL CHAIR: Dr. Toyohiro Chikyo (NIMS, Japan)

### **INTERNATIONAL ADVISORY BOARD:**

Dr. Wolfgang Schrof (BASF, Germany) Prof. Klaus Stöwe (University of Chemnitz, Germany) Dr. Toyohiro Chikyow (NIMS, Japan) Prof. Stefano Curtarolo (Duke University) Prof. Calum Drummond (RMIT University) Prof. Kenjiro Fujimoto (Tokyo University of Science, Japan) Dr. Martin L. Green (NIST, U.S.A.) Prof. Brian E Hayden (University of Southampton, U.K.) Dr. Jason Hattrick-Simpers (NIST, U.S.A.) Dr. Alamgir Karim (University of Akron) Prof. Hideomi Koinuma (NIMS, Japan) Prof. Jochen Lauterbach (University of South Carolina, U.S.A.) Prof. Alfred Ludwig (Ruhr-Universität Bochum, Germany) Prof. Wilhelm F. Maier (Saarland University, Germany) Prof. Ulrich S. Schubert (Friedrich-Schiller-Universität Jena, Germany) Prof. Ichiro Takeuchi (University of Maryland) Prof. Seong Ihl Woo (KAIST, Korea)

### LOCAL ORGANIZING COMMITTEE

Chair: Prof. Kenjiro Fujimoto (Tokyo University of Science, Japan) Dr. Toyohiro Chikyo (NIMS, Japan) Prof. Yuji Matsumoto (Tohoku Univ.) Prof. Shingo Maruyama (Tohoku Univ.) Prof. Shintaro Yasui (Tokyo Inst. Tech.) Prof. Ryota Takahashi (Tokyo Univ.) Prof. Akihisa Aimi (Tokyo Univ. Science) Dr. Isao Ohkubo (NIMS)

## **General Information**

## Program overview

	2nd October		3rd October		4th October		5th October		
9:00			Registration		Registration		Registration		9:00
9:30			Opening remarks		S-1		I-09		9:30
			PL-1				O-14		
10:00			PI -2		I-07		O-15		10:00
10.30					O-10	E	O-16	<u> </u>	10.30
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11:00			I-01		Break		I-10		11:00
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### **Practical Information**

### **Badge Policy**

All persons wishing to present their research and/or attend the workshop sessions or evening events are required to register and must wear their meeting badges at all times. Anyone not wearing badge will be ask to leave the event rooms immediately.

### Oral presentations guidelines

In order to avoid unnecessary delays during the presentation, authors need to prepare before the presentation so that they can quickly and easily transition from one story to another. All conversations are limited to the time stated in the program including the setup time to connect the laptop. In this workshop, we will use HDMI cable with priority. (VGA cable is also available)

### Poster presentation guidelines

Attendees can mount their poster from morning until before the formal presentation Please remove your poster the same day.

We expect authors to be present at their posters for discussion with attendees during the session. <u>Organizing committee and International</u> <u>advisory board members will select the best poster presentation.</u> The winners will be announced during the banquet.

### WIFI access

Meeting place hotel Mielparque Yokohama provides WIFI environment. You can use the following login and password.

Login :

Password :

Please refrain from transmitting and receiving huge data as much as possible.

### Coffee and Lunch breaks

Coffee breaks (between sessions and before starting afternoon session) are organized for COMBI2018 attendees in the workshop room. Please use lunch at Chinatown or nearby restaurants.

### Workshop venue

#### **Mielparque Yokohama**

Yamashita-cho 16, Naka-ku, Yokohama, Kanagawa 231-0023, Japan



In case of using Minatomirai line, Exit 4 of Motomachi-Chukagai station is the shortest route to the hotel.

### Local transportation

#### From Tokyo International Airport (HANEDA, HND) <Case 1> Haneda Airport Station -> Yokohama Station (Keikyu Line) Yokohama station -> Motomachi-Chukagai station (Yokohama Minatomirai Railway; Minatomirai line) Motomachi-Chukagai station (Exit No.4) -> Mielparque Yokohama (about 1 min by walk) (Total: $\sim 60$ min.) <Case 2> Haneda Airport -> Yokohama Ningyonoie Mae (English name; Yokohama Doll Museum) (stop in front of Mielparque Yokohama) Bus operation: Keikyu Limousine bus Operation schedule: http://hnd-bus.com/airport/h-yamashita/ (Total: ~30 min) From Narita International Airport (NARITA, NRT) Narita Airport Station -> Yokohama Station <Case 1> (East Japan Railway; Narita Express) Yokohama station -> Motomachi-Chukagai station (Yokohama Minatomirai Railway; Minatomirai line) Motomachi-Chukagai station -> Mielparque Yokohama (about 1 min by walk) (Total: ~100~120 min.) <Case 2> Narita Airport Station -> Yokohama City Air Terminal; YCAT (Limousine bus) YCAT -> Yokohama station (about 350 m by walk) Yokohama station -> Motomachi-Chukagai station (Yokohama Minatomirai Railway; Minatomirai line) Motomachi-Chukagai station (Exit No.4) -> Mielparque Yokohama (about 1 min by walk) (Total: ~ 120 min.)

#### **Additional Information**

From Yokohama station to Yamashita Park you can also use the boat's bus (SEE BASS).

https://www.yokohama-cruising.jp/img/pamphlet\_english.pdf

## Registration

	Early Bird	On-site		
	~ 30 <sup>th</sup> September	1 <sup>st</sup> October ~		
Regular attendee (Company)	¥60,000	¥70,000		
Regular attendee (Academic)	¥50,000	¥60,000		
Student	¥25,000	¥30,000		

The registration fee includes a welcome party and a banquet. In addition, credit card transaction fee (3%) is also included.

### **Caution**!

Credit card payment at the venue cannot be done.

Only cash will be handled at the venue.

## Welcome reception (including registration fee)

Welcome reception will be held at October 2, 2018 in "Rainbow room" (7 th floor) in conference venue from 6pm-9pm with registration.



## **Conference Tour (Excursion) – Kamakura trip**

From the end of the 12th century to the middle of the 14th century, the shogunate was placed in Kamakura and occupied one of the most important positions in Japanese politics.

A special guide will guide you on the history and landscape of Kamakura. Those who have chosen to participate in Excursion on the Registration site can participate. This excursion departs by bus at around 1 pm in front of the workshop venue. In Kamakura we will explore by the guide of Kamakura Welcome Guide Association.

KWGA; http://kamakurawelcome.guide/en/

We leave Kamakura around 5 pm and arrive at the workshop venue around 6 o'clock in the evening.

Participation fee is 3,000 JPY. Please pay at reception desk.

## **Banquet (including registration fee)**

Our local organizing committee plans night cruising at Yokohama Port. The departure time is 18:30. Please get on board so as not to be late.



### About prohibition of photography etc.

Our organizing committee will prohibit the following within the presentation hall.

- photographing presentation slides and posters
- video recording presentation slides and posters

However, this is not the case when the organizing committee takes pictures for publicity.

### **Scientific Program**

3<sup>rd</sup> October 2018

9:00~ Registration desk open

9:15~9:25 Opening Remarks General chair: Dr. Toyohiro Chikyow

1<sup>st</sup> Session Chair: Dr. Martin L. Green (NIST)

9:25~10:00 Plenary Talk (PL-1)

Accelerating Materials Development through Rapid Analysis of Experimental Data using Machine Learning based Tools

John Perkins<sup>a</sup>, Andriy Zakutayev<sup>a</sup>, Marcus Schwarting<sup>a,b</sup>, Caleb Phillips<sup>b</sup>, Robert White<sup>a,b</sup>, Kristin Munch<sup>b</sup>, Bill Tumas<sup>a</sup>

<sup>a</sup> Materials Science Center, National Renewable Energy Laboratory, USA <sup>b</sup> Computational Sciences Center, National Renewable Energy Laboratory, USA

10:00~10:35 Plenary Talk (PL-2) Overview of Materials Informatics Project in Japan Satoshi ITOH National Institute for Materials Science, Japan

10:35~10:50 Break

#### 2<sup>nd</sup> Session Chair: Prof. Ichiro Takeuchi (Maryland Univ.)

10:50~11:15 Invited Talk (I-01) Introduction to the Chinese MGI and high-throughput materials research Zhongpei Feng<sup>a</sup>, Ge He<sup>a</sup>, Jie Yuan<sup>a,b</sup>, and Kui Jin<sup>a,b</sup> <sup>a</sup> Institute of Physics, Chinese Academy of Sciences, China <sup>b</sup> Key Laboratory for Vacuum Physics, University of Chinese Academy of Sciences, China

11:15~11:40 Invited Talk (I-02)

Attaining the Promise of MGI by Combining HiTp Experimentation with Artificial Intelligence

Apurva Mehta<sup>a</sup>, Jason Hattrick-Simpers<sup>b</sup> and Chris Wolverton<sup>c</sup> *<sup>a</sup> SLAC National Accelerator Lab, USA <sup>b</sup> NIST, USA <sup>c</sup> Northwestern University, USA* 

11:40~12:00 Oral Presentation (O-01)
Next Generation Materials Genome Research at NIST
Martin L. Green, James Warren, Brian DeCost, Jason Hattrick-Simpers, A. Gilad
Kusne and Zachary Trautt
National Institute of Standards and Technology, USA

12:00~12:20 Oral Presentation (O-02)

Building a Collaboratory for High-Throughput Experimental Materials Science Zachary Trautt<sup>a</sup>, Martin Green<sup>a</sup>, Jason Hattrick-Simpers<sup>a</sup>, A. Gilad Kusne<sup>a</sup>, Brian DeCost<sup>a</sup>, John Perkins<sup>b</sup>, Andriy Zakutayev<sup>b</sup> and Caleb Phillips<sup>b</sup> <sup>a</sup> National Institute of Standards and Technology, USA <sup>b</sup> National Renewable Energy Laboratory, USA

12:20~13:50 Lunch

<u>3rd Session Chair: Prof. Brian E. Hayden (University of Southampton)</u> <u>& Prof. Shintaro Yasui (Tokyo Institute of Technology)</u>

13:50~14:15 Invited Talk (I-03)

Materials Discovery Materials discovery in multinary thin film and nanoparticle libraries

Alfred Ludwig

Institute for Materials and ZGH (Center for Interface-Dominated High Performance Materials), Ruhr-University Bochum, Germany

#### 14:15~14:40 Invited Talk (I-04)

Combinatorial sputter coating technique combined with materials informatics for development of thermal related energy materials

Masahiro Goto

National Institute for Materials Science, Japan

#### 14:40~15:00 Oral Presentation (O-03)

#### High Throughput Experimental Materials Database

Andriy Zakutayev<sup>a\*</sup>, Nick Wunder<sup>b</sup>, Marcus Schwarting<sup>a,b</sup>, John D. Perkins<sup>a</sup>, Robert White<sup>a,b</sup>, Kristin Munch<sup>b</sup>, William Tumas<sup>a</sup>, Caleb Phillips<sup>b</sup>

<sup>a</sup> Materials Science Center, National Renewable Energy Laboratory, USA

<sup>b</sup> Computational Sciences Center, National Renewable Energy Laboratory, USA.

15:00~15:20 Oral Presentation (O-04)

#### Autonomous X-ray Diffraction System for Accelerated Combinatorial Phase Diagram Mapping

Brian DeCost<sup>a</sup>, Heshan Yu<sup>b</sup>, Xiaohang Zhang<sup>b</sup>, Seunghun Lee<sup>b</sup>, Yangang Liang<sup>b</sup>, Jason Hattrick-Simpers<sup>a</sup>, Ichiro Takeuchi<sup>b</sup>, and A. Gilad Kusne<sup>a,b</sup>

<sup>a</sup> National Institute of Standards and Technology, USA

<sup>b</sup> University of Maryland, USA

15:20~15:40 Oral Presentation (O-05)

# Scanning Kelvin Probe and Scanning Droplet Cell Microscopy as Complementary Screening Tools for Combinatorial Material Libraries

Achim Walter Hassel<sup>a,b</sup>, Silvia Huber<sup>a</sup> and Jan Philipp Kollender<sup>b</sup>

<sup>a</sup> Christian Doppler Laboratory for Combinatorial Oxide Chemistry at TIM, Johannes Kepler University Linz, Austria

<sup>b</sup> Institute for Chemical Technology of Inorganic Materials (TIM), Johannes Kepler University Linz, Austria

15:40~15:55 Break

#### <u>4<sup>th</sup> Session Chair: Prof. Seong Ihl Woo (KAIST)</u> & Prof. Ryota Takahashi (The University of Tokyo)

15:55~16:20 Invited Talk (I-05) Combinatorial Experimentation and Machine Learning for Materials Discovery Ichiro TAKEUCHI Department of Materials Science and Engineering, University of Maryland, USA

16:20~16:45 Invited Talk (I-06)

Material Development by Integrated Approach of Combinatorial Experiments, High-Throughput ab-initio Calculation and Explainable AI (XAI)

Yuma Iwasaki <sup>a,b</sup>

<sup>a</sup> System Platform Research Laboratories, NEC Corporation, Japan <sup>b</sup> PRESTO, JST, Japan

16:45~17:05 Oral Presentation (O-06)

An Inter-Laboratory High Throughput Experimental Materials Study of Sn-Zn-Ti-O

J. R. Hattrick-Simpers<sup>a</sup>, A. Zakutayev<sup>b</sup>, J. Perkins<sup>b</sup>, S. C. Barron<sup>c</sup>, Z. T. Trautt<sup>a</sup>, N. Nguyen<sup>a</sup>, K. Choudhary<sup>a</sup>, C. Phillips<sup>b</sup>, A. G. Kusne<sup>a</sup>, F. Yi<sup>a</sup>, A. Mehta<sup>d</sup>, M. L. Green<sup>a</sup>

<sup>a</sup> National Institute of Standards and Technology (NIST), USA

<sup>b</sup> National Renewable Energy Laboratory (NREL), USA

<sup>c</sup> Charles Stark Draper Laboratory, USA

<sup>d</sup> SLAC National Accelerator Laboratory, USA

17:05~17:25 Oral Presentation (O-07)

Combinatorial Material and Device Optimisation of Tunable Dielectrics for Smart Microwave and Millimetre-Wave Systems

Brian E. Hayden<sup>a,b</sup>, Ioanna Bakaimi<sup>a</sup>, Kees De Groot<sup>a</sup>, Xingli He<sup>a</sup> Ian Reaney<sup>c</sup>, and Samuel Guerin<sup>b</sup>

<sup>a</sup> University of Southampton, U.K.

<sup>b</sup> Ilika Technologies, U.K.

<sup>°</sup> Department of Engineering Materials, University of Sheffield, U.K.

17:25~17:45 Oral Presentation (O-08)

Electrocatalytic compositional mapping of copper-alloy libraries for sensor applications

Andrei Ionut Mardare <sup>a,b</sup>, Isabella Pötzelberger <sup>a</sup>, Cezarina Cela Mardare <sup>c</sup>, Achim Walter Hassel<sup>a,b,c</sup>

<sup>a</sup> Institute for Chemical Technology of Inorganic Materials, Johannes Kepler University Linz, Austria

<sup>b</sup> Competence Centre for Electrochemical Surface Technology (CEST), Austria

<sup>°</sup> Christian Doppler Laboratory for Combinatorial Oxide Chemistry, Austria

17:45~18:05 Oral Presentation (O-09)

**Polymer Blend and Composite Library Preparation from Hot Organic Solutions** Ezgi Dogan Guner, Zihao Qu, Mike McBride, Guoyan Zhang, Elsa Reichmanis, Martha Grover, Carson Meredith

School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, USA

18:05~18:15 Group photo

#### 18:15~20:05 Poster Presentation

#### 4<sup>th</sup> October 2018

9:00~ Registration desk open

#### 5<sup>th</sup> Session Chair: Dr. Toyohiro Chikyow (NIMS)

9:15~9:50 Special Talk (S-1)

General and personal history of combinatorial materials science and catalysis Wilhelm Maier

Chemistry Department, Saarland University, Germany

9:50~10:15 Invited talk (I-07)

High-throughput experimentation in polymer research: From new pharmapolymers to nanoparticle libraries and new battery materials

Ulrich S. Schubert a,b,c,d

<sup>a</sup> Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Germany

<sup>b</sup> Jena Center for Soft Matter (JCSM), Friedrich Schiller University Jena, Germany

<sup>°</sup> Center for Energy and Environmental Chemistry Jena (CEEC), Germany

<sup>d</sup> Max Planck Institute of Colloids and Interfaces, Germany

10:15~10:35 Oral presentation (O-10)

High-Throughput Synthesis and Characterization of Eu Doped  $Sr_xBa_{2-x}SiO_4$  Thin Film Phosphors

Sara Frost<sup>a</sup>, Samuel Guérin<sup>a</sup>, Brian E. Hayden<sup>a,b</sup>, Jean-Philippe Soulié<sup>a</sup>, and Chris Vian

<sup>a</sup> Ilika Technologies, U.K.

<sup>b</sup> University of Southampton, U.K.

10:35~10:55 Oral presentation (O-11)

**The Synthesis of Single-chip Superconductor Library with Continuous Tc Gradient** Jie Yuan<sup>a</sup>, Zhongpei Feng<sup>a</sup>, Ge He<sup>a</sup>, Xu Zhang<sup>a</sup>, Jongmoon Shin<sup>b</sup>, Ichiro Takeuchi<sup>b</sup> and Kui Jin<sup>a</sup>

<sup>a</sup> The Institute of Physics, Chinese Academy of Sciences, China

<sup>b</sup> Department of Materials Science and Engineering, University of Maryland, USA

10:55~11:10 Break

6th Session Chair: Prof. Jochen Lauterbach (University of South Carolina)

11:00~11:35 Invited talk (I-08)

**Topological data analysis of magnetic domain structure** M Kotsugi<sup>a,b</sup> *<sup>a</sup> Tokyo University of Science, Japan* 

<sup>b</sup> Mf I, NIMS, Japan

11:35~11:55 Oral presentation (O-12) Catalyst Discovery via High Throughput Screening and Machine Learning: Ru based

Catalysts for Low Temperature Ammonia Decomposition

Katie McCullough<sup>a</sup>, Travis Williams<sup>a</sup> and Jochen Lauterbach<sup>a</sup>

<sup>a</sup> Department of Chemical Engineering, University of South Carolina, USA

11:55~12:15 Oral presentation (O-13)

Combinatorial Search for IrO<sub>2</sub>-RuO<sub>2</sub>-TiO<sub>2</sub> system for Chlorine Evolution Electrode Catalyst

Junpei Sakurai<sup>a</sup>, Shingo Takagi<sup>a</sup>, Masashi Miyamoto<sup>a</sup>, Kimihiko Sugiura<sup>a</sup>, Chiemi Oka <sup>a</sup>, Mizue Mizoshiri<sup>b</sup>, Seiichi Hata<sup>a</sup>

<sup>a</sup> Nagoya University, Japan

<sup>b</sup> Nagaoka University of Technology, Japan

12:15~13:15 Lunch

13:15~18:15 Excursion

18:30~20:00 Banquet

5<sup>th</sup> October 2018

9:00~ Registration desk open

7th Session Chair: Dr. Jason Hattrick-Simpers (NIST)

9:15~9:40 Invited talk (I-09)

Materials informatics for thermal functional material

Junichiro Shiomi<sup>a,b,c</sup>

<sup>a</sup> The University of Tokyo, Japan

<sup>b</sup> National Institute for Materials Science, Japan

<sup>c</sup> RIKEN Center for Advanced Intelligence Project, Japan

9:40~10:00 Oral presentation (O-14)

Development of unexplored materials accelerated by first-principle calculations and informatics

Isao Ohkubo <sup>a,b,c,d</sup>, and Takao Mori <sup>a,c</sup>

<sup>a</sup> Center for Functional Sensor & Actuator, Research Center for Functional Materials, National Institute for Materials Science (NIMS), Japan

<sup>b</sup> Center for Materials Research by Information Integration (CMP), Research and Services Division of Materials Data and Integrated System (MaDIS), National Institute for Materials Science (NIMS), Japan

<sup>c</sup> International Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), Japan <sup>d</sup> IST PRESTO, Japan

<sup>d</sup> JST-PRESTO, Japan

10:00~10:20 Oral presentation (O-15)

High-throughput modelling of defect structures of oxide-ion conductors

Naoto Kitamura<sup>®</sup>, Naoya Ishida<sup>®</sup> and Yasushi Idemoto<sup>®</sup>

<sup>a</sup> Faculty of Science and Technology, Tokyo University of Science, Japan

10:20~10:40 Oral presentation (O-16)

# Automated Synthesis of Semiconductor Nanocrystals: A Multidimensional Study on the Influence of Mixing Using High Throughput Methodologies

Ahmed M. Salaheldin and Doris Segets Institute of Particle Technology (LFG), Interdisciplinary Center for Functional Particle

Systems (FPS), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany

10:40~10:55 Break

8th Session Chair: Prof. Alfred Ludwig (Ruhr-Universität Bochum)

10:55~11:20 Invited talk (I-10)

Accelerated Materials Discovery Powered by Machine Learning

Ryo Yoshida <sup>a,b</sup>

<sup>a</sup> The Institute of Statistical Mathematics, Japan

<sup>b</sup> National Institute for Materials Science, Japan

11:20~11:40 Oral presentation (O-17)

Automated Synthesis and Characterization of Photoluminescence Quantum Yield of Semiconductor Nanocrystals

Ahmed M. Salaheldin and Doris Segets

Institute of Particle Technology (LFG), Interdisciplinary Center for Functional Particle Systems (FPS), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany 11:40~12:00 Oral presentation (O-18)

**High-throughput Mapping of Organic Thin Film Libraries by Microbeam GI-WAXS** Shingo Maruyama<sup>a</sup>, Yusuke Takagawa<sup>a</sup>, Kana Ouchi<sup>a</sup>, Tomoyuki Koganezawa<sup>b</sup> and Yuji Matsumoto<sup>a</sup>

<sup>a</sup> Tohoku University, Sendai, Miyagi 980-8579, Japan <sup>b</sup> Japan Synchrotron Radiation Research Institute (JASRI), Japan

12:00~12:20 Oral presentation (O-19)

## Electrochemical evaluation of thin film negative electrodes for lithium ion batteries formed by combinatorial sputtering

Tomoya Kishi<sup>a</sup>, Kazushi Hayashi<sup>a</sup>, Takashi Segi<sup>b</sup> and Kenji Koga<sup>b</sup>

<sup>a</sup> Applied Physics Research Laboratory, Kobe Steel, LTD., Japan

<sup>b</sup> Material Solutions Division, Kobelco Research Institute, INC., Japan

12:20~13:30 Lunch

9th Session Chair: Prof. Kenjiro Fujimoto (Tokyo University of Science)

13:30~13:50 Oral presentation (O-20)

Combinatorial High-Throughput Optical Screening of High Performance for Li-air and Li ion Battery

Seong Ihl Woo<sup>a,b</sup>, Sung Hyeon Park<sup>a</sup>, Young Jin Jun<sup>a</sup>, Seung Yong Lee<sup>a</sup>, Hee Sang Lee <sup>a,b</sup>

<sup>a</sup> Korea Advanced Institute of Science and Technology, Chemical and Biomolecular Engineering, Republic of Korea <sup>b</sup> Harmony, N28, Republic of Korea

13:50~14:10 Oral presentation (O-21) **High-Throughput Experimentation at the CSIRO** Shaun Howard<sup>a</sup>, and Ben Muir<sup>a</sup> <sup>a</sup> CSIRO, Melbourne, Australia

14:10~14:35 Invited talk (I-11)

Towards the paradigm shift in materials research from simple nano to integrated nano, and to smart combinatorial drone technology

Hideomi Koinuma <sup>a,b,c</sup>, Masashi Kawasaki <sup>d</sup>, Mikk Lippmaa <sup>d</sup>, Kenji Itaka <sup>e</sup>, Nobuyuki Matsuki<sup>f</sup>

<sup>a</sup> SCT, Inc.,Japan

<sup>b</sup> Tokyo Institute of Technology, Japan

° National Institute for Materials Science, Japan

<sup>d</sup> The University of Tokyo, Japan

<sup>e</sup> Hirosaki University, Japan

<sup>f</sup> Kanagawa University, Japan

14:35~14:50 Closing Remarks & Next Workshop Information Local organizing committee chair: Prof. Kenjiro Fujimoto

### Poster Presentation < Sponsored by ACS Combinatorial Science >

3<sup>rd</sup> October 2018 18:05-20:05

Session chair: <u>Dr. Jason Hattrick-Simpers (NIST) & Dr. Isao Ohkubo (NIMS)</u> <u>& Prof. Wilhelm F. Maier (Saarland University)</u>

P-01

#### The Materials Data Curation System

Zachary Trautt<sup>a</sup>, Alden Dima<sup>a</sup>, Kevin Brady<sup>a</sup>, Benjamin Long<sup>a</sup>, Chandler Becker<sup>a</sup>, Raymond Plante<sup>a</sup>, Guillaume Sousa Amaral<sup>a</sup>, Xavier Schmitt<sup>a</sup>, Adrien Catel<sup>a</sup>, Pierre Francois Rigodiat<sup>a</sup>, Philippe Dessauw<sup>a</sup>

<sup>a</sup> National Institute of Standards and Technology, USA

#### P-02

Development of Ge diffusion barrier layer at  $CeF_3/Ge$  interface by combinatorial method

Takahiro Nagata<sup>a,b</sup>, Shigenori Ueda<sup>c,d</sup> Yoshiyuki Yamashita<sup>a</sup>, Asahiko Matsuda<sup>e</sup>, and Toyohiro Chikyow<sup>e</sup>

<sup>a</sup> International Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), Japan

<sup>b</sup> JST, PRESTO, Japan

° Synchrotron X-ray Station at SPring-8, NIMS, Japan

<sup>d</sup> Research Center for Advanced Measurement and Characterization, NIMS, Japan

<sup>e</sup> Materials Data & Integrated System (MaDIS), NIMS, Japan

#### P-03

#### Combinatorial nitrogen gradients in sputtered thin films

Yanbing Han<sup>a,b</sup>, Bethany Matthews<sup>a,c</sup>, Dennice Roberts<sup>a,d</sup>, Kevin R. Talley<sup>a,e</sup>, Sage R. Bauers<sup>a</sup>, Craig Perkins<sup>a</sup>, Qun Zhang<sup>b</sup>, Andriy Zakutayev<sup>a</sup>

<sup>a</sup> Materials Science Center, National Renewable Energy Laboratory, USA

<sup>b</sup> Department of Materials Science, Fudan University, China

° Department of Physics, Oregon State University, USA

<sup>d</sup> Department of Mechanical Engineering, University of Colorado at Boulder, USA

<sup>°</sup> Department of Metallurgical and Materials Engineering, Colorado School of Mines, USA

#### P-04

#### Development of multi-dot array fabrication system for materials informatics

Naoto Oki<sup>a</sup>, Kohei Maruyama<sup>a</sup>, Natsumi Takikawa<sup>a</sup>, Tadashi Nishio<sup>a</sup>, Shun Konno<sup>a</sup>, Masaki Sekine, Tohru Higuchi<sup>a</sup>, Takuo Ohkochi<sup>b</sup> and Masato Kotsugi<sup>a\*</sup>

<sup>a</sup> Tokyo University of Science, Japan

<sup>b</sup> SPring-8, Japan

#### P-05

Combinatorial Exploration of Metal Alloying in Iron Vanadate for Photoelectrochemical Water Splitting

Lydia H. Wong, Wilman Septina, Mengyuan Zhang, Thi Hiep Nguyen, Ying Fan Tay, Joel Ming Rui Tan

School of Materials Science & Engineering, Nanyang Technological University, Singapore

#### Combinatorial fabrication and spectroscopy of binary thin film alloys

Tadashi Nishio<sup>a</sup>, Masahiro Yamamoto<sup>a</sup>, Naoaki Yamanaka<sup>a</sup>, Tomoyuki Kadono<sup>a</sup>, Takuo Ohkochi<sup>b</sup> and Masato Kotsugi<sup>a</sup>

<sup>a</sup> Graduate school of Tokyo University of Science, Japan <sup>b</sup> Spring-8, Japan

#### P-07

# High Throughput Synthesis of Perovskite Films for Multi-Dimensional Material Optimization

Ahmed M. Salaheldin, Elisabeth Reinhardt, Monica Distaso, Doris Segets and Wolfgang Peukert

Institute of Particle Technology (LFG), Interdisciplinary Center for Functional Particle Systems (FPS), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany

#### P-08

#### Combinatorial Discovery of Ultra-large Grain Growth of Vacuum Deposited PTCDI-Cn Thin Films

Yusuke Takagawa<sup>a</sup>, Shingo Maruyama<sup>a</sup>, Tomoyuki Koganezawa<sup>b</sup> and Yuji Matsumoto

<sup>a</sup> Tohoku University, Japan

<sup>b</sup> Japan Synchrotron Radiation Research Institute (JASRI), SPring-8, Japan

#### P-09

#### High throughput research of tunable superconductivity in FeSe

Zhongpei Feng<sup>a,b</sup>

<sup>a</sup> Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, China

<sup>b</sup> University of Chinese Academy of Sciences, China

#### P-10

#### Screening of bismuth oxide-based novel oxide ion conductor by combining highthroughput synthesis method with Materials Informatics

Masato Matsubara, Akitoshi Suzumura, Nobuko Ohba, Shin Tajima and Ryoji Asahi Toyota Central R&D Laboratories, Inc., Japan

#### P-11

# Combinatorial screening of ternary Li-alloy anodes for high performance lithium-ion batteries

Yaoyu Ren<sup>a</sup>, Kedar Manandhar<sup>a</sup>, Drew Stasak<sup>a</sup>, Huilong Hou<sup>a</sup>, Jing Xu<sup>b</sup>, Joonho Koh<sup>b</sup>, John P. Lemmon<sup>b</sup>, Ichiro Takeuchi<sup>a</sup>

<sup>a</sup> University of Maryland, Department of Materials Science and Engineering, USA <sup>b</sup> NICE America Research Inc., USA

#### P-12

# Development of evaluation substrate for biocompatibility combinatorial evaluation of high formable shape memory alloys

Kaname CHIZUWA<sup>a</sup>, Chiemi OKA<sup>a</sup>, Seiichi HATA<sup>a</sup>, Junpei SAKURAI<sup>a</sup>

<sup>a</sup> Department of Micro-Nano Mechanical Science and Engineering, Nagoya University, Japan

Candidate thermoelectric materials exploration of perovskite-type  $Ca_{1-x}A_xMn_{1-y}B_yO_{3-d}$  (*A*; La, Bi, Y, Sr,

B; Ni, Ti, V, x = y = 0.02) using solution processing

Yusuke YAMADA<sup>a</sup>, Minoru GIBU<sup>a</sup>, Shogo YOSHIDA<sup>a</sup>, Yuki YAMAGUCHI<sup>a</sup>, Akihisa AIMI<sup>a</sup>, Keishi NISHIO<sup>b</sup> and Kenjiro FUJIMOTO<sup>a</sup>

<sup>a</sup> Faculty of Science and Technology, Tokyo University of Science, Japan

<sup>b</sup> Department of Materials Science of Technology, Tokyo University of Science, Japan

#### P-14

# Electrochemical Property of Tungsten Trioxide-Nickel-Oxide Library in an Acidic Solution

Jun-Seob Lee<sup>a</sup>, Andrei Ionut Mardare<sup>b,c</sup>, Cezarina Cela Mardare<sup>b,c</sup> and Achim Walter Hassel<sup>b,c,\*</sup>

<sup>a</sup> Competence Centre for Electrochemical Surface Technology (CEST), Austria

<sup>b</sup> Institute for Chemical Technology of Inorganic Materials, Johannes Kepler University Linz, Austria

<sup>°</sup> Christian Doppler Laboratory for Combinatorial Oxide Chemistry at ICTAS, Johannes Kepler University Linz, Austria

#### P-15

#### Chemical delithiation of LiMn<sub>1/3</sub>Ni<sub>1/3</sub>Co<sub>1/3</sub>O<sub>2</sub> using various acid solutions

Koyo YASUMOTO<sup>a</sup>, Akihisa AIMI<sup>a</sup>, Yuta SHIMONISHI<sup>b</sup>, Nobuo YAMAMOTO<sup>b</sup>, Shuhei YOSHIDA<sup>b</sup>, Shun OKIJIMA<sup>b</sup> and Kenjiro FUJIMOTO<sup>a</sup>

<sup>a</sup> Department of Pure and Applied Chemistry, Faculty of Science and Technology, Tokyo University of Science, Japan <sup>b</sup> DENSO CORPORATION Japan

<sup>b</sup> DENSO CORPORATION, Japan

#### P-16

#### Combinatorial Development of Copper Based Bulk Elastocaloric Materials

Jun Cui<sup>a,b</sup>, Gaoyuan Ouyang<sup>a</sup>, Emry Farmer<sup>a</sup>, XuboLiu<sup>b</sup>, and Ichiro Takeuchi<sup>c</sup>

<sup>a</sup> Iowa State University, Materials Science & Engineering Department, USA

<sup>b</sup> Ames Laboratory, Materials Science and Engineering Division, USA

<sup>c</sup> University of Maryland, Materials Science & Engineering Department, USA

#### P-17

#### Exploring of the Zirconium Oxide Based Afterglow Phosphors

Hiroaki TAKAHASHI, Kenjiro FUJIMOTO and Akihisa AIMI Faculty of Science and Technology, Tokyo University of Science, Japan

#### P-18

#### Combinatorial study on piezoresponse by in-situ Synchrotron x-ray diffraction

Shintaro Yasui<sup>a,b</sup>, Yoshitaka Ehara<sup>c</sup>, Takahisa Shiraishi<sup>c</sup>, Takao Shimizu<sup>c</sup>, Hiroshi Funakubo<sup>c</sup>, Mitsuru Itoh<sup>b</sup>, Yasuhiko Imai<sup>d</sup>, Hiroo Tajiri<sup>d</sup>, Osami Sakata<sup>c,e</sup>, Ichiro Takeuchi<sup>a</sup>

<sup>a</sup> Dept. of MSE, University of Maryland, USA

<sup>b</sup> MSL, Tokyo Institute of Technology, Japan

° Dept. of MSE, Tokyo Institute of Technology, Japan

<sup>d</sup> Japan Synchrotron Radiation Research Institute/SPring-8, Japan

<sup>e</sup> National Institute for Materials Science/SPring-8, Japan

#### Automatic Materials Design using Monte Carlo Tree Search with Bayesian Learning

Thaer M. Dieb<sup>a,b,c</sup>, Zhufeng Hou<sup>b</sup> and Koji Tsuda<sup>a,b,c</sup>

<sup>a</sup> National Institute for Materials Science, Japan

<sup>b</sup> The University of Tokyo, Japan

° Canter for Advanced Intelligence Project, RIKEN, Japan

#### P-20

#### Automation of Crystal Structure Refinement Using the Rietveld Analysis

Akihisa Aimi<sup>a</sup> and Kenjiro Fujimoto<sup>a</sup>

<sup>a</sup> Department of Pure and Applied Chemistry, Faculty of Science and Technology, Tokyo University of Science, Japan

#### P-21

# Accelerated data collection and analysis of synchrotron X-ray powder diffraction and X-ray absorption fine structure measurements

Kenjiro FUJIMOTO<sup>a</sup>, Akihisa AIMI<sup>a</sup> and Shingo MARUYAMA<sup>b</sup>

<sup>a</sup> Department of Pure and Applied Chemistry, Faculty of Science and Technology, Tokyo University of Science, Japan

<sup>b</sup> Department of Applied Chemistry, School of Engineering, Tohoku University, Japan

#### P-22

#### Scientific Data Infrastructure for Combinatorial Materials Science

Sigurd Thienhaus, Lars Banko and Alfred Ludwig

Ruhr-University Bochum, Institute for Materials, Germany

#### P-23

#### **Materials Data Specification and Block Chain based Data Copyright Protection** Quan Qian<sup>a,b</sup>, Pengfei Li<sup>b</sup> and Rui Zhang<sup>b</sup>

<sup>a</sup> School of Computer Engineering & Science, Shanghai University, P.R. China <sup>b</sup> Materials Genome Institute, Shanghai University, P.R. China

#### P-24

# Virtual Boundary Detection with Deep Learning Method for Materials Image Segmentation

Lai Chuanbin<sup>a</sup>, Yuexing Han<sup>b,a</sup>, and Quan Qian<sup>a,c</sup>

 <sup>a</sup> School of Computer Engineering & Science, Shanghai University, P.R. China
 <sup>b</sup> Shanghai Institute for Advanced Communication and Data Science, Key Laboratory of Shanghai University, P.R. China
 <sup>c</sup> Materials Genome Institute, Shanghai University, P.R. China

#### P-25

# Virtual Boundary Detection with Deep Learning Method for Materials Image Segmentation

Atsushi Yamamoto, Kunihiro Kihou and Chul-Ho Lee

National Institute of Advanced Industrial Science and Technology, Japan

## Toward High-throughput Mechanical Study of Square Membranes using Spherical Tip Indentation

Euimin Cheong, Donghyun Park, Injun Oh, Kyunghoon Kim and Dongwoo Lee School of Mechanical Engineering, Sungkyunkwan University, Korea

#### P-27

#### Prediction of Formation Energies of Interstitial Atoms in HCP Crystals

Daegun You<sup>a</sup>, Minsoo Joo<sup>a</sup>, Won-Yong Shin<sup>b</sup>, Keonwook Kang<sup>c</sup> and Dongwoo Lee<sup>a</sup> <sup>a</sup> School of Mechanical Engineering, Sungkyunkwan University, Korea

<sup>b</sup> Department of Computer Science and Engineering, Dankook University, Korea

<sup>°</sup> Department of Mechanical Engineering, Yonsei University, Seoul, Korea

#### P-28

#### Design of a High-throughput System with Replaceable Measurement Modules to Investigate Combinatorial Metallic Glasses

Donghyun Park, Daegun You, Euimin Cheong, Injun Oh, Haechan Jo, Kyunghoon Kim and Dongwoo Lee

School of Mechanical Engineering, Sungkyunkwan University, Korea

#### P-29

Properties Prediction of Inorganic Material Using Machine Learning with Experimental and Computational Hybrid Database

Chia-Yung Jui<sup>a</sup>, Wen-Jay Lee<sup>a</sup>

<sup>a</sup> National Center for High-performance Computing, National Applied Research Laboratories, Taiwan (R.O.C.)

#### P-30

## Combinatorial sputter coating technique applied for thermoelectric thin films of bismuth telluride

Michiko Sasaki, Xu Yibin, Yukihiro Isoda, Yoshikazu Shinohara and Masahiro Goto *National Institute for Materials Science, Japan* 

#### P-31

Vision-based Alignment of Small Scale Specimens for High-Throughput Experiments Haechan Jo, Donghyun Park, Euimin Cheong, Injun Oh, and Dongwoo Lee School of Mechanical Engineering, Sungkyunkwan University, Korea

#### P-32

#### Accelerated Deovolopment of Magnet Alloy With Decreased Critical Materials

R. T. Ott<sup>a,b</sup>, E. Simsek<sup>a</sup>, F. Meng<sup>a</sup>, R. Chaudry<sup>a</sup>, and I. C. Nlebedim<sup>b</sup> <sup>a</sup> Ames Laboratory (USDOE), Division of Materials Science and Engineering, Ames, IA, USA

<sup>b</sup> Ames Laboratory (USDOE), Critical Materials Institute, Ames, IA, USA

Combinatorial Synthesis & High Throughput Characterization of NiTi-based Shape Memory Alloy Libraries for Thermoelastic Cooling

Naila Al Hasan<sup>a</sup>, Huilong Hou<sup>a</sup>, Suchismita Sarkar<sup>b</sup>, Fang Ren<sup>b</sup>, Tieren Gao<sup>a</sup>, Jonathan Counsell<sup>c</sup>, A. Gilad Kusne<sup>d</sup>, Apurva Mehta<sup>b</sup>, Ichiro Takeuchi<sup>a</sup>

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