

Table of Contents

Preface	4
Cooperating Organizations	5
Organizing Committees	6
Conference Information	7
Schedule Overview	10
Venue Map	11
Time Table (Symposium Oral Sessions)	12
Time Table (Symposium Poster Sessions)	13
Floor Guide	14
Plenary Lectures	23
Cluster Keynotes	37
Cluster A-I	
A. Fundamentals for Materials	99
A-1 Local Atomic Structure Analysis on the Active Center of Functional Materials	100
A-2 Hydrogen in Functional Materials	106
A-3 Recent Advances in Computational Materials Science: Bridging Computations and Experiments	111
A-4 Neutrons for Materials Research	113
B. New Trend of Materials Research	117
B-1 Data-Centric Science for Materials Research	118
B-2 Materials Integration: Fusion of Materials Science and Experiments through Data Science	122
B-3 Mathematical Materials Science -Mathematical Approaches for Materials Designs in the Data Driven Society	124
B-4 Topological Materials Science for Innovative Functions	128
C. Novel Structural Materials Based on New Principles	131
C-1 Fundamental Issues of Structural Materials	132
C-2 Mille-feuille Structured Light-weight Materials	136
C-3 Hard and Tough Ceramics	139
C-4 Tough Polymers	143
D. Advanced Electronic Materials	147
D-1 2D Layered Materials	148
D-2 Novel Concepts of Electronic Materials Inspired from Complementary and Competing Fields	153
D-3 Science and Technology of Superconductivity	155
D-4 [5th E&J BLS] Wide-bandgap and 2-dimensional Materials	164

E. Magnet and Spintronics	167
E-1 New Aspects of Understanding Magnetic Materials	168
E-2 Spin Conversion Phenomena in Spin Orbit Materials	172
E-3 Quantum State in Low Symmetry Environment Probed by Advanced Spin Polarized Quantum Beam	175
F. Energy	179
F-1 Battery Materials for Sustainability	180
F-2 Catalysis and Catalyst Materials for Energy and Environment	185
F-3 Advancements in Thermoelectric Materials and Applications	191
F-4 Synchrotron X-ray Probes for Mesoscale Materials Science	199
G. Materials for Smart Systems	203
G-1 In-field Molecules for Next-generations Flexible Electronics	204
G-2 [5th E&J BLS] Materials Frontier for Transparent Advanced Electronics	206
G-3 Perovskite and Metal Halide Materials Based Photovoltaics and Optoelectronics	212
G-4 Plasmonic Materials: from Fundamentals to Applications	216
G-5 Synchrotron X-ray Characterization of Function Material Thin Films and Fine Particles	220
H. Green Technology and Processing	223
H-1 Advanced Water Science and Technology	224
H-2 Plasma-Based Synthesis, Processing and Characterization of Materials for Energy and Environment	232
H-3 [5th E&J BLS] Advanced Functional Oxides: Processing, Characterization and Devices	236
H-4 A3+ Lead-free Piezoelectric Materials and Applications	242
H-5 Intelligent Material Processes with Low Environmental Load and Energy Consumption	245
I. Biopolymers	251
I-1 Bio-based Polymers	252
I-2 Environmentally Degradable Polymers	253
I-3 Biodegradable Polymers for Biomedical Applications	256
Sponsors and Exhibitors	inside back cover

Preface

Scope of MRM2019

Materials science is rapidly expanding across the traditional boundaries of physics, chemistry, biology, and earth science for achieving Sustainable Development Goals (SDGs). There are many issues in the world that need to be solved on a global scale. The future of humankind and the development of a sustainable society depend on the development of new materials and their integration in the energy-water-food nexus. To achieve this requires integration of modeling, basic theory, high throughput materials science, and advanced characterization in a new approach to science and technology.

The MRM2019 is intended to offer a venue to materials researchers from different disciplines to discuss recent scientific developments and applications of advanced materials for the SDGs. There are many new opportunities for invention and brilliant materials research, and implementation of new materials or processes, in fields far from our individual disciplines. Intensive discussions among participants with different background are expected to bring innovative ideas and strategic development for next generation materials research. The meeting will also provide active opportunities for young researchers to discuss their research projects, thus extending the groundwork for a successful network and for synergetic collaborations. A dialogue across the following topic areas with notable scientists who are world experts with diverse backgrounds in materials research will be constructed. Each topic area is of both current and future interest and must be addressed to achieve sustainability. The organizers welcome participants who are interested in materials research and expect an exciting and fruitful discussion.



Hideo HOSONO (Prof. Tokyo Tech)
Chairperson of MRM2019



Atsushi SUZUKI (Prof. YNU)
General Secretary of MRM2019

Conference Information

Date	December 10 (Tue.) – 14 (Sat.)
Conference Site	Industry & Trade Center (Yokohama Symposia): Trade-0~3 Workpia Yokohama: Work-1~8 Hotel Mielparque Yokohama: Miel-1~5 Hotel Monterey Yokohama: Mont-1~5 Kanagawa Kenmin Hall: Ken-1~2 Yokohama City Port Opening Memorial Hall: Port-1~4
Registration Desk	Marineria, Industry & Trade Center 1F (Trade-0)
Registration Hours	December 10 (Tue.) 11:00–18:00 December 11 (Wed.) 8:30–18:30 December 12 (Thu.) 8:30–18:30 December 13 (Fri.) 8:30–18:00
Welcome Party	December 10 (Tue.) 19:00–20:30 Work-1 & 2 (Oshidori & Kujaku), Workpia Yokohama, 2F
Banquet	December 12 (Thu.) 19:00–21:00 Rose Hotel Yokohama
Exhibition	Marineria, Industry & Trade Center 1F (Trade-0)
Exhibition Hours	December 11 (Wed.) 12:00–20:30 December 12 (Thu.) 9:30–18:00 December 13 (Fri.) 9:30–16:00
Emergency Contact	Secretariat for MRM2019 Email: info_mrm2019@jmru.org Phone: 070-3157-6169 (Connected only for the conference period , Dec. 9 - Dec. 14, 2019)
Plenary Lectures	<p>[Plenary Session 1] December 10 (Tue.) 15:00–15:40 Place: Trade-1 (Industry & Trade Center) Hans-Joachim Freund (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany)</p> <p>[Plenary Session 2] December 10 (Tue.) 15:50–16:30 Place: Trade-1 (Industry & Trade Center) Jean-Marie Tarascon (College de France, France)</p> <p>[Plenary Session 3] December 10 (Tue.) 16:40–17:20 Place: Trade-1 (Industry & Trade Center) Marius Grundman (Universitat Leipzig Institut fur Experimentelle Physik, Germany)</p> <p>[Plenary Session 4] December 10 (Tue.) 17:30–18:20 Place: Trade-1 (Industry & Trade Center) Shinji Tsuneyuki (University of Tokyo, Japan)</p>

[Plenary Session 5]

December 11 (Wed.) 13:00–13:40

Place: Ken-1 (Small Hall, Kanagawa Kenmin Hall)

Easo P George (Oak Ridge National Laboratory and the University of Tennessee, USA)

[Plenary Session 6]

December 12 (Thu.) 13:00–13:40

Place: Ken-1 (Small Hall, Kanagawa Kenmin Hall)

David S. Ginley (NREL Fellow, USA)

[Plenary Session 7]

December 13 (Fri.) 13:00–13:40

Place: Ken-1 (Small Hall, Kanagawa Kenmin Hall)

Michael Coey (Trinity College Dublin, Ireland)

Cluster Keynote
Place: Ken-1 (Small Hall, Kanagawa Kenmin Hall)

A Cluster December 11 (Wed.) 16:30–18:30

B Cluster December 12 (Thu.) 9:30–12:00

C Cluster December 13 (Fri.) 14:00–16:00

D Cluster December 12 (Thu.) 14:00–16:00

E Cluster December 11 (Wed.) 9:30–12:05

F Cluster December 12 (Thu.) 16:30–18:30

G Cluster December 13 (Fri.) 9:30–11:50

H Cluster December 11 (Wed.) 14:00–16:00

I Cluster December 13 (Fri.) 16:30–18:00

Oral Presentation
December 11 (Wed.)

Oral Session 1, Oral Session 2, Oral Session 3

December 12 (Thu.)

Oral Session 4, Oral Session 5, Oral Session 6

December 13 (Fri.)

Oral Session 7, Oral Session 8, Oral Session 9

December 14 (Sat.)

Oral Session 10

Poster Session
Place: Trade-0 (Marineria)
Poster 1 December 11 (Wed.)

Symposium F-2, H-1

Set up 9:00–11:30

Poster Display 12:00–13:00

Removal Until 14:00

Poster 2 December 11 (Wed.)

Symposium A-3, B-4, C-1, D-1, D-2, D-3, D-4, E-2, F-3, H-1

Set up 16:00–19:00

Poster Display 19:00–20:30

Removal Until 21:00

Poster 3 December 12 (Thu.)

Symposium B-1, B-3, H-2, H-3, H-4

Set up 9:00–14:00

Poster Display 14:00–15:30

Removal Until 16:00

Poster 4 December 12 (Thu.)
 Symposium A-1, A-4, C-2, C-3, E-1, G-2
 Set up 16:00–16:30
 Poster Display 16:30–18:00
 Removal Until 18:30

Poster 5 December 13 (Fri.)
 Symposium E-3, F-1, I-1, I-2
 Set up 9:00–14:00
 Poster Display 14:00–15:30
 Removal Until 16:30

Poster 6 December 13 (Fri.)
 Symposium A-2, C-4, F-4, G-1, G-3, G-4, G-5, H-5
 Set up 17:00–19:00
 Poster Display 19:00–20:30
 Removal Until 21:00

Tutorial December 10 (Tue.) Only in Japanese

[Tutorial Session 1]

12:00–12:50 Work-1 (Oshidori, Workpia Yokohama)

What we can know from first-principles quantum calculations

Speaker: Toshio Kamiya (Laboratory for Materials and Structures (MSL), Institute of Innovative Research (IIR), Tokyo Institute of Technology (Tokyo Tech))

Chair: Shunichi ARISAWA (National Institute for Materials Science)

[Tutorial Session 2]

12:55–13:45 Work-1 (Oshidori, Workpia Yokohama)

Sparse modeling for Materials informatics

Speaker: Yasuhiko Igarashi (Graduate School of Frontier Sciences, The University of Tokyo)

Chair: Shunichi ARISAWA (National Institute for Materials Science)

[Tutorial Session 3]

13:50–14:40 Work-1 (Oshidori, Workpia Yokohama)

Materials Informatics and Physics Informatics by Interpretable Machine Learning

Speaker: Yuma Iwasaki (Central Research Laboratories, NEC Corporation)

Chair: Shunichi ARISAWA (National Institute for Materials Science)

[Tutorial Session 4]

12:00–12:50 Work-2 (Kujaku, Workpia Yokohama)

How to start using neutron and muon at J-PARC

Speaker: Kazuki Ohishi (Comprehensive Research Organization for Science and Society (CROSS))

Chair: Takaaki AOKI (Institute for Information Management and Communication, Kyoto University)

[Tutorial Session 5]

12:55–13:45 Work-2 (Kujaku, Workpia Yokohama)

Application of Synchrotron Radiation Research and Use of SPring-8

Speaker: Toyohiko Kinoshita (Japan Synchrotron Radiation Research Institute (JASRI))

Chair: Takaaki AOKI (Institute for Information Management and Communication, Kyoto University)

[Tutorial Session 6]

13:50–14:40 Work-2 (Kujaku, Workpia Yokohama)

New trend in materials science by integration of quantum beam analysis and machine learning

Speaker: Tetsuro Ueno (National Institutes for Quantum and Radiological Science and Technology)

Chair: Takaaki AOKI (Quantum Beam Science Research Directorate, Institute for Information Management and Communication, Kyoto University)

Schedule Overview

	Dec. 10 (Tue.)	Dec. 11 (Wed.)	Dec. 12 (Thu.)	Dec. 13 (Fri.)	Dec. 14 (Sat.)		
8:30		8:30–18:30 Registration	8:30–18:30 Registration	8:30–18:30 Registration			
9:00		Oral Session 1 9:00–11:30 A-1 / A-3 / A-4 / B-1 / B-3 / B-4 / C-1 / D-1 / D-3 / D-4 / F-2 / F-3 / G-2 / H-1 / H-2 / H-3 9:30–12:05 E Cluster Keynote	Oral Session 4 9:00–11:30 A-1 / A-4 / C-1 / C-2 / C-3 / C-4 / D-1 / D-2 / D-3 / D-4 / E-3 / F-1 / F-3 / G-2 / G-3 / H-1 / H-2 / H-3 / H-4 / H-5 9:30–12:00 A-2 9:30–12:00 B Cluster Keynote	Oral Session 7 9:00–11:30 A-2 / A-4 / B-2 / B-3 / C-2 / C-3 / C-4 / D-1 / D-3 / E-1 / E-3 / F-1 / F-3 / F-4 / H-2 / H-3 / H-4 / H-5 / I-1 / I-2 / I-3 9:30–12:00 A-2 / B-2 / B-3 / C-3 / F-4 9:30–11:50 G Cluster Keynote	9:00–11:30 Oral Session 10 D-3 / I-3		
10:00							
11:00	11:00–18:00 Registration						
12:00	12:00–12:50 Tutorial 1 Tutorial 4	12:00–13:00 Poster Session 1					
13:00	12:55–13:45 Tutorial 2 Tutorial 5	13:00–13:40 Plenary 5 Easo P George	13:00–13:40 Plenary 6 David S. Ginley	13:00–13:40 Plenary 7 Michael Coey			
14:00	13:50–14:40 Tutorial 3 Tutorial 6	14:00–16:00 Oral Session 2 A-1 / A-3 / A-4 / B-1 / B-3 / B-4 / C-1 / C-3 / D-1 / D-3 / D-4 / E-2 / E-3 / F-2 / F-3 / G-2	14:00–16:00 Oral Session 5 A-1 / A-2 / A-4 / B-2 / C-1 / C-2 / C-3 / C-4 / E-1 / E-3 / F-1 / F-3 / G-2 / G-3 / G-4 / H-1 / H-5 / I-2	14:00–16:00 Oral Session 8 A-2 / B-2 / B-3 / D-1 / D-3 / E-1 / F-3 / F-4 / G-1 / G-2 / G-3 / G-4 / G-5 / H-3 / H-4 / H-5 / I-3			
15:00	14:50–15:00 Opening Hideo Hosono Tokyo, Tech. / Chairperson of MRM2019 15:00–15:40 Plenary 1 Hans-Joachim Freund	14:00–16:00 H Cluster Keynote	14:00–16:00 D Cluster Keynote 14:00–15:30 Poster Session 3	14:00–16:00 C Cluster Keynote 14:00–15:30 Poster Session 5			
16:00	15:50–16:30 Plenary 2 Jean-Marie Tarascon						
17:00	16:40–17:20 Plenary 3 Marius Grundman 17:30–18:20 Plenary 4 Shinji Tsuneyuki	16:30–18:30 Oral Session 3 B-1 / B-3 / B-4 / C-1 / C-3 / D-1 / D-3 / D-4 / E-2 / E-3 / F-2 / F-3 / G-2 / H-1 / H-2 / H-3 / H-4 / H-5 16:30–18:30 A Cluster Keynote	16:30–18:30 Oral Session 6 B-1 / B-2 / B-3 / C-1 / C-4 / D-1 / D-2 / D-3 / D-4 / E-3 / G-3 / G-4 / H-1 / H-2 / H-3 / H-4 / H-5 / I-2 / I-3 16:30–18:30 F Cluster Keynote	16:30–18:30 Oral Session 9 A-2 / B-2 / B-3 / C-3 / C-4 / D-3 / E-1 / F-3 / F-4 / G-1 / G-2 / G-3 / G-4 / G-5 / H-5 16:30–18:30 I Cluster Keynote			
18:00	18:20–18:30 Short Message		16:30–18:00 Poster Session 4				
19:00	19:00–20:30 Welcome Reception	19:00–20:30 Poster Session 2	19:00–21:00 Banquet	19:00–20:30 Poster Session 6			
20:00							

Venue Map



1 Industry & Trade Center (Yokohama Symposia)

- Trade-1 Main Hall (9F)
- Trade-2 Room 803+804 (8F)
- Trade-3 Special Meeting Room (8F)
- Trade-0 Marina (1F)
- Registration (1F)
- Exhibition (1F)
- Poster session (1F)

2 Workpia Yokohama

- Work-1 OSHIDORI (2F)
- Work-2 KUJAKU (2F)
- Work-3 Room 201 (2F)
- Work-4 YAMAAYURI (3F)
- Work-5 KAMOME (3F)
- Work-6 ICHOU (3F)
- Work-7 Room 302 (3F)
- Work-8 Room 301 (3F)

3 Kanagawa Kenmin Hall

- Ken-1 Small Hall (1F)
- Ken-2 Conference Room (large) (6F)

4 HOTEL Monterey Yokohama

- Mont-1 Hall MAPLE (1F)
- Mont-2 Hall KENSINGTON (2F)
- Mont-3 RICHMOND (2F)
- Mont-4 AISAI • ICHOU (2F)
- Mont-5 Hall VICTORIA (3F)

5 HOTEL Mielparque Yokohama

- Miel-1 Cherie (2F)
- Miel-2 Etoile (2F)
- Miel-3 Kohaku (2F)
- Miel-4 Ruby (2F)
- Miel-5 Hissui (2F)

6 Yokohama City Port Opening Memorial Hall

- Port-1 Room 1 (1F)
- Port-2 Room 6 (2F)
- Port-3 Room 7 (2F)
- Port-4 Room 9 (2F)

7 Rose Hotel Yokohama

- Banquet (The Grand Rose Ballroom 2F)

Time Table (Symposium Oral Sessions)

Symposium Time Room	Day 1 Dec. 11			Day 2 Dec. 12			Day 3 Dec. 13			Day 4 Dec. 14	
	Oral Session 1	Oral Session 2	Oral Session 3	Oral Session 4	Oral Session 5	Oral Session 6	Oral Session 7	Oral Session 8	Oral Session 9	Oral Session 10	
A-1	9:00-11:20 Mont-5	14:00-16:00 Mont-5		9:00-11:20 Mont-5	14:00-15:30 Trade-1						
A-2			16:30-18:30 A Cluster Keynote Ken-1	9:30-12:15 Ken-2	14:00-16:30 Ken-2		9:30-11:45 Ken-2	14:00-15:40 Ken-2	16:30-17:30 Ken-2		
A-3	9:00-11:35 Mont-2	14:00-15:55 Mont-2		9:00-11:15 Mont-2	14:00-16:15 Mont-2		9:00-11:35 MH-5				
A-4	9:00-11:30 MH-4	14:00-15:55 MH-4		9:30-12:00 B Cluster Keynote Ken-1	14:00-16:10 Port-3	16:30-18:20 Port-3	9:30-11:30 Port-3	14:00-15:50 Port-3	16:30-18:30 Port-3		
B-1	9:00-11:30 MH-1	14:00-16:00 MH-1	16:30-18:30 MH-1			16:30-18:30 Port-1					
B-2				9:30-12:00 B Cluster Keynote Ken-1	14:00-16:10 Port-3	16:30-18:20 Port-3	9:30-11:30 Port-3	14:00-15:50 Port-3	16:30-18:30 Port-3		
B-3	9:00-11:20 Work-3	14:00-16:00 Work-3	16:30-18:40 Work-3			16:30-18:30 Port-2	9:30-11:40 Port-2	14:00-15:50 Port-2	16:30-18:00 Port-2		
B-4	9:00-11:30 Work-8	14:00-16:00 Work-8	16:30-18:30 Work-8								
C-1	9:00-11:20 Mont-1	14:00-16:10 Mont-1	16:30-18:30 Mont-1	9:00-11:20 Mont-1	14:00-15:55 Mont-1	16:30-17:30 Mont-1					
C-2				9:00-11:30 Work-8	14:00-16:00 Work-8		9:00-11:30 Work-8	14:00-16:00 C Cluster Keynote Ken-1	16:30-18:25 Work-1		
C-3		14:00-16:05 Work-6	16:30-18:25 Work-6	9:00-11:25 Work-6	14:00-15:45 Work-6	16:30-18:30 Work-6	9:30-11:50 Port-1	14:00-16:00 Ken-1	16:30-18:30 Port-1		
C-4				9:00-11:30 Work-4	14:00-16:10 Work-4	16:30-18:30 Work-4	9:00-11:40 Work-4	14:00-16:00 Work-4	16:30-18:30 MH-5		
D-1	9:00-11:30 Work-4	14:00-16:00 Work-4	16:30-18:30 Work-4	9:00-11:30 Mont-3	16:30-18:30 Mont-3		9:00-11:30 Mont-3	14:00-16:00 Mont-3			
D-2				9:00-11:30 Work-7	14:00-16:00 Work-7	16:30-18:30 Work-7					
D-3	9:00-11:40 Trade-1	14:00-16:00 Trade-1	16:30-18:30 Trade-1	9:00-12:10 Work-1	16:30-18:30 Work-1	16:30-18:30 Work-1	9:00-12:10 Ken-1	14:00-16:00 Work-1	16:30-18:30 Work-1	9:00-12:20 Work-1	
D-3 (2)							9:00-12:10 Work-6	14:00-16:00 Work-6	16:30-18:30 Work-6		
D-4	9:00-11:30 Trade-3	14:00-16:00 Trade-3	16:30-18:30 Trade-3	9:00-11:30 MH-5	16:30-18:30 Work-6						
E-1	9:30-12:00 E Cluster Keynote Ken-1	14:00-16:20 MH-5	16:30-18:35 MH-5		14:00-16:00 Mont-3		9:00-11:30 Mont-4	14:00-16:00 Mont-4	16:30-17:30 Mont-4		
E-2											
E-3	14:00-16:00 Trade-2	16:30-18:35 Trade-2	9:00-11:30 Trade-3	14:00-16:05 Trade-3	16:30-18:55 Trade-3	9:00-11:45 Trade-1					

Symposium Time Room	Day 1 Dec. 11			Day 2 Dec. 12			Day 3 Dec. 13			Day 4 Dec. 14
	Oral Session 1	Oral Session 2	Oral Session 3	Oral Session 4	Oral Session 5	Oral Session 6	Oral Session 7	Oral Session 8	Oral Session 9	Oral Session 10
F-1							9:00-11:20 Work-5			
F-2	9:00-12:15 Work-5	14:00-16:10 Work-5	16:30-18:40 Work-5		14:00-16:05 Work-5	16:30-18:30 F Cluster Keynote Ken-1	9:00-12:05 Work-2	14:00-16:10 Work-2	16:30-18:45 Work-2	
F-3	9:00-12:05 Work-2	14:00-16:00 Work-2	16:30-18:30 Work-2	9:00-12:05 Trade-1	14:00-16:10 Work-2		9:30-11:40 Port-4	14:00-16:00 Port-4	16:30-18:20 Port-4	
F-4										
G-1								14:00-16:20 Work-3	16:30-18:30 Work-3	
G-2	9:00-11:30 Work-1	14:00-16:00 Work-1	16:30-18:30 Work-1	9:00-11:30 MH-2	14:00-16:00 MH-2	16:30-18:30 MH-1	9:30-12:00 G Cluster Keynote Ken-1	14:00-16:00 Trade-1	16:30-17:30 Trade-1	
G-3				9:00-11:30 MH-1	14:00-16:00 MH-1	16:30-18:05 MH-5		14:00-16:00 MH-3	16:30-18:40 MH-3	
G-4								14:00-16:05 Work-4	16:30-18:00 Work-4	
G-5								14:00-16:10 Work-8	16:30-18:20 Work-8	
H-1	9:00-11:45 MH-3	16:30-18:30 MH-3	9:00-12:25 MH-3	14:00-16:00 MH-3	16:30-18:40 MH-3					
H-2	9:00-11:30 Mont-3	14:00-16:00 Mont-3	16:30-18:30 Work-3	9:00-11:30 Work-3	16:30-18:30 Work-3	9:00-11:30 Work-3				
H-3	9:00-11:20 MH-2	14:00-16:00 H Cluster Keynote Ken-1	16:30-18:30 MH-2	9:00-11:25 Work-2	16:30-18:30 Work-2	9:00-11:30 MH-2				
H-4				9:00-11:00 MH-4	16:30-18:45 MH-4	9:00-11:00 MH-4				
H-5				16:30-18:35 Mont-5	9:00-11:30 Trade-2	14:00-16:00 Trade-2	9:00-11:20 Mont-5	14:00-16:00 Work-5	16:30-18:25 Work-5	
I-1										
I-2				14:00-16:00 Mont-4	16:30-18:30 Mont-4					
I-3								14:00-15:52 Mont-2	16:30-18:00 I Cluster Keynote Ken-1	9:00-11:29 Work-3

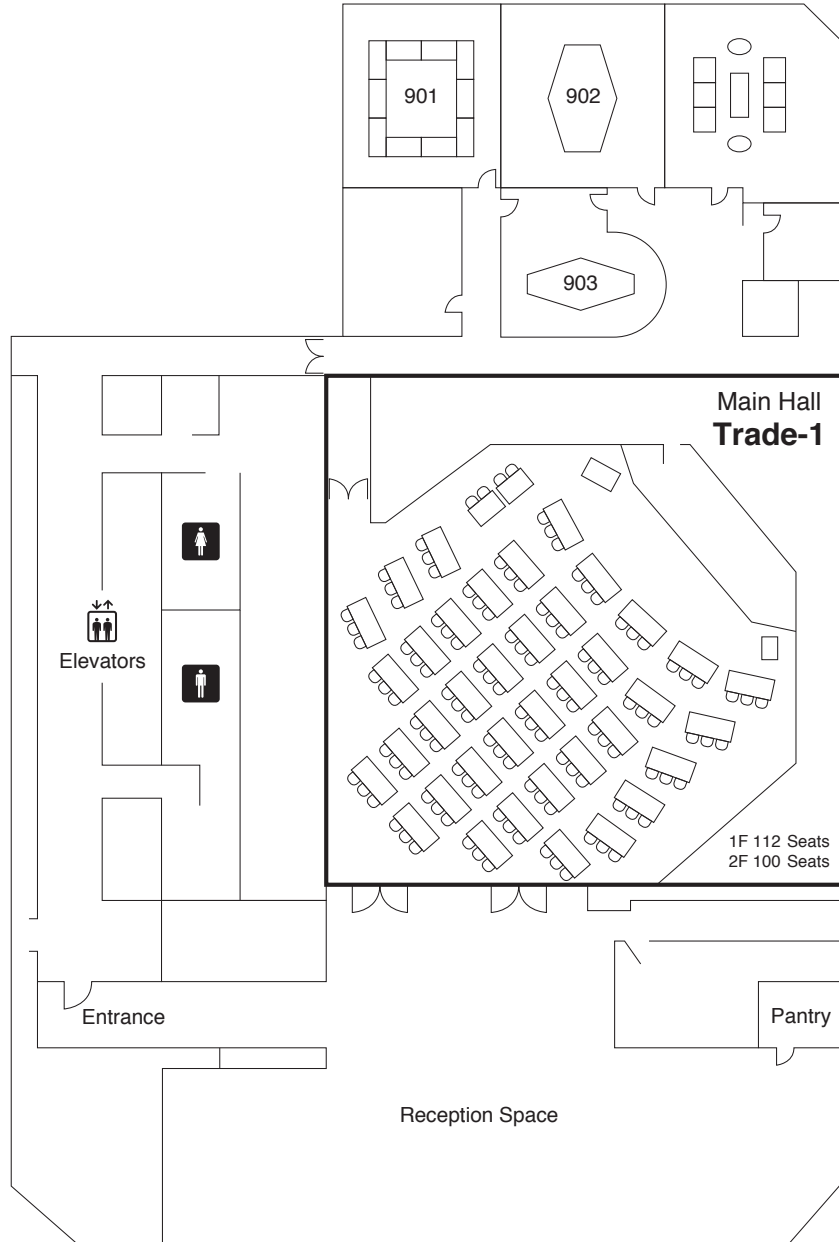
Time Table (Symposium Poster Sessions)

	Dec. 11		Dec. 12		Dec. 13		
	Poster 1	Poster 2	Poster 3	Poster 4	Poster 5	Poster 6	
	11:30-14:00	19:00-20:30	14:00-15:30	16:30-18:00	14:00-15:30	19:00-20:30	
A-1				○			A-1
A-2						○	A-2
A-3		○					A-3
A-4				○			A-4
B-1			○				B-1
B-2							B-2
B-3			○				B-3
B-4		○					B-4
C-1		○					C-1
C-2				○			C-2
C-3				○			C-3
C-4						○	C-4
D-1		○					D-1
D-2		○					D-2
D-3		○					D-3
D-4		○					D-4
E-1				○			E-1
E-2		○					E-2
E-3					○		E-3
F-1					○		F-1
F-2	○						F-2
F-3		○					F-3
F-4						○	F-4
G-1						○	G-1
G-2				○			G-2
G-3						○	G-3
G-4						○	G-4
G-5						○	G-5
H-1	○	○					H-1
H-2			○				H-2
H-3			○				H-3
H-4			○				H-4
H-5						○	H-5
I-1					○		I-1
I-2					○		I-2
I-3							I-3

Floor Guide

Industry & Trade Center Yokohama Symposia

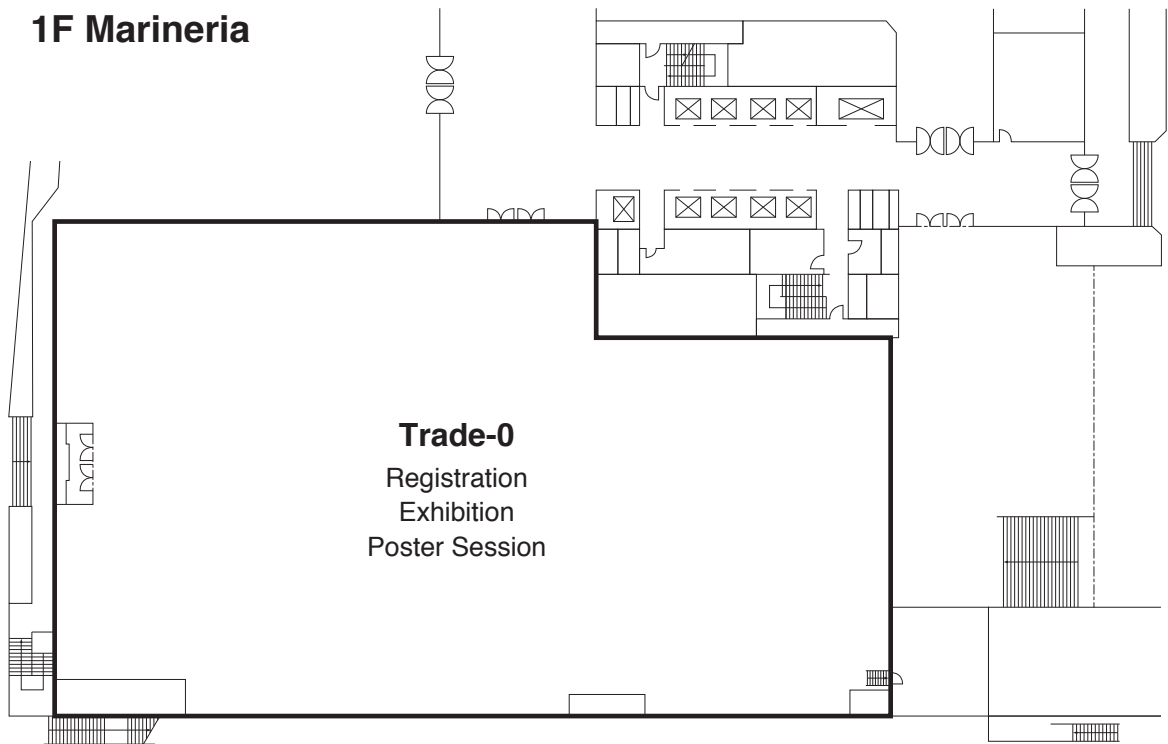
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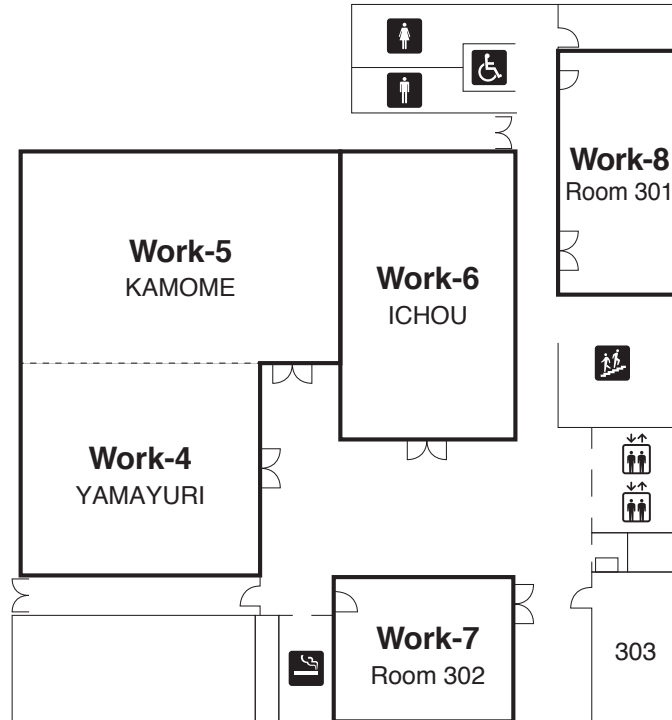


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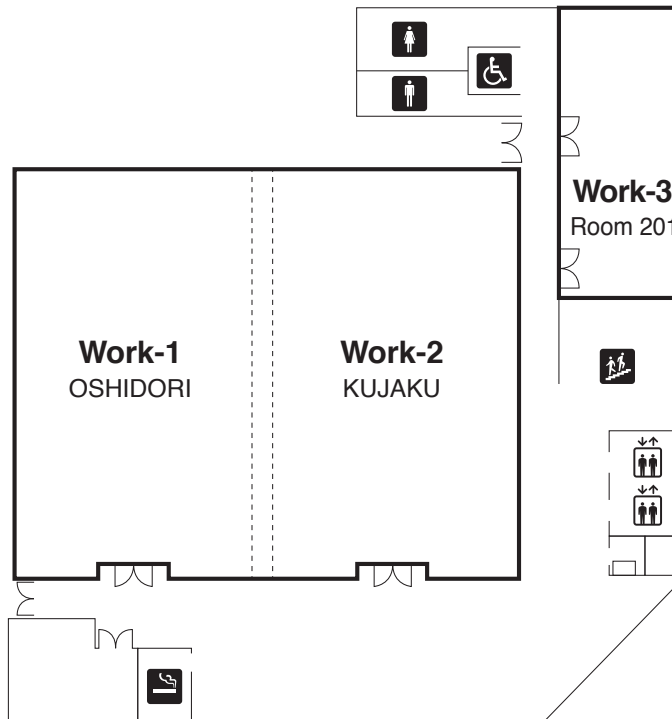


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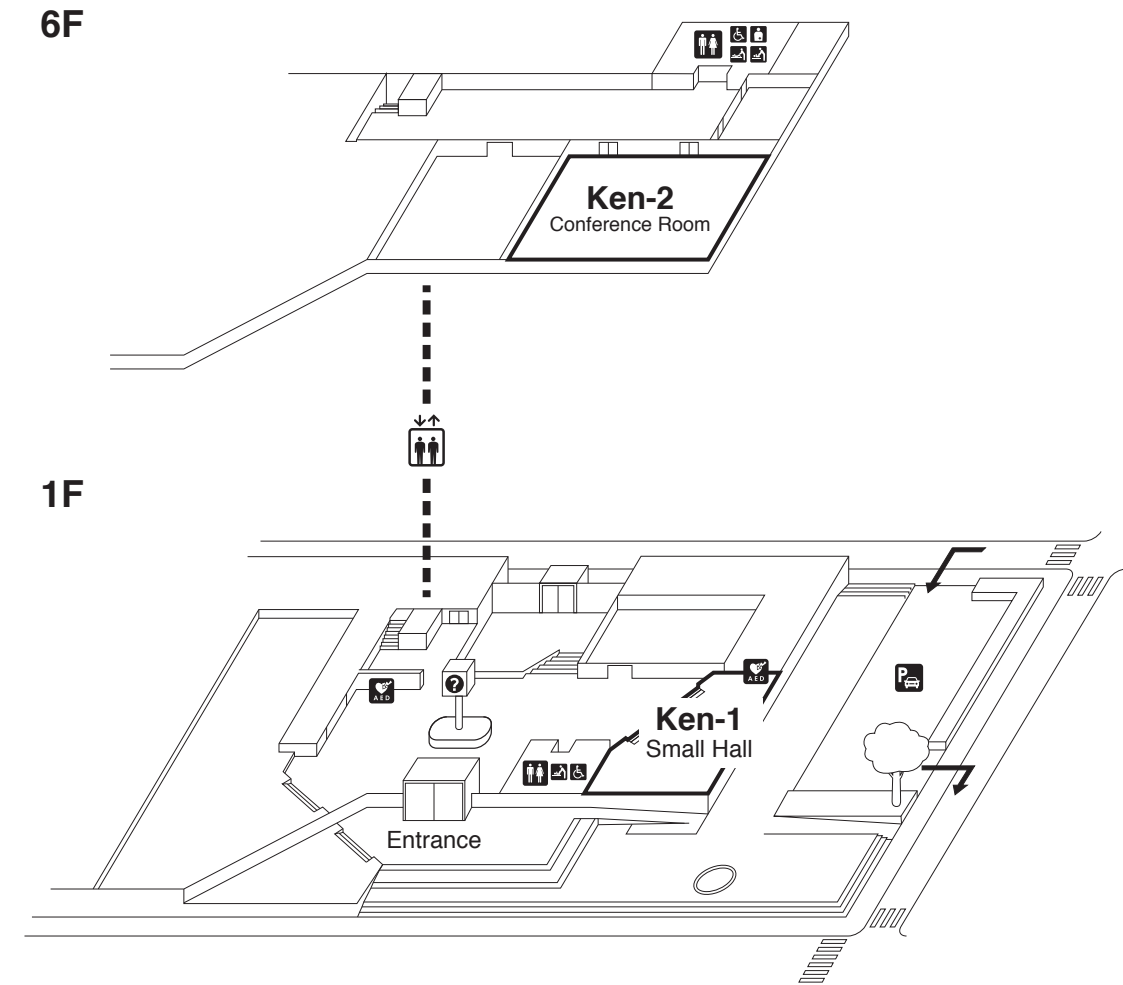
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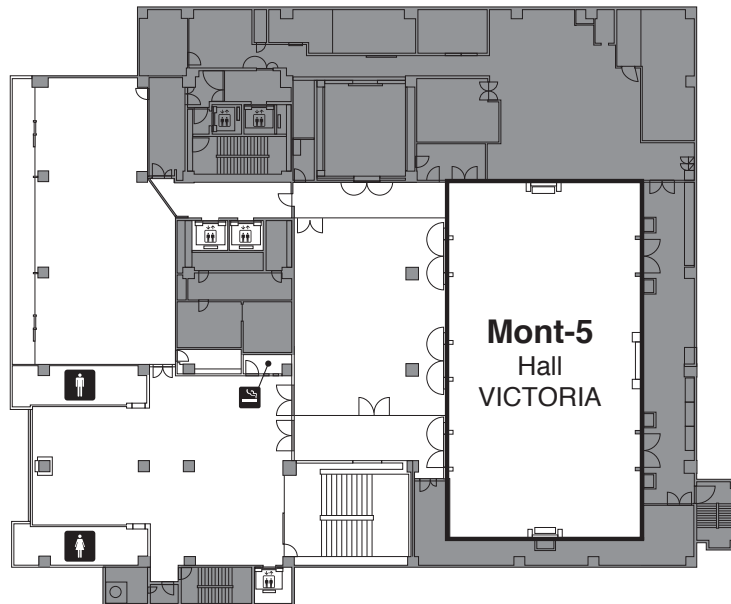


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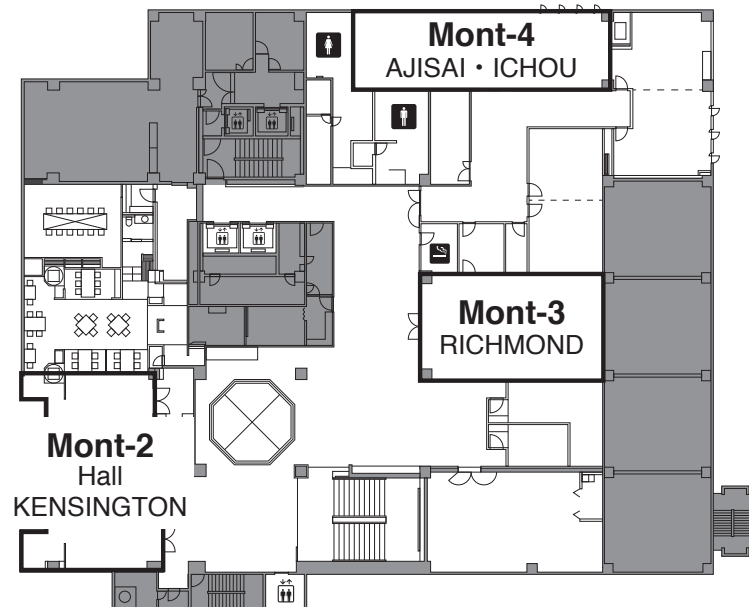


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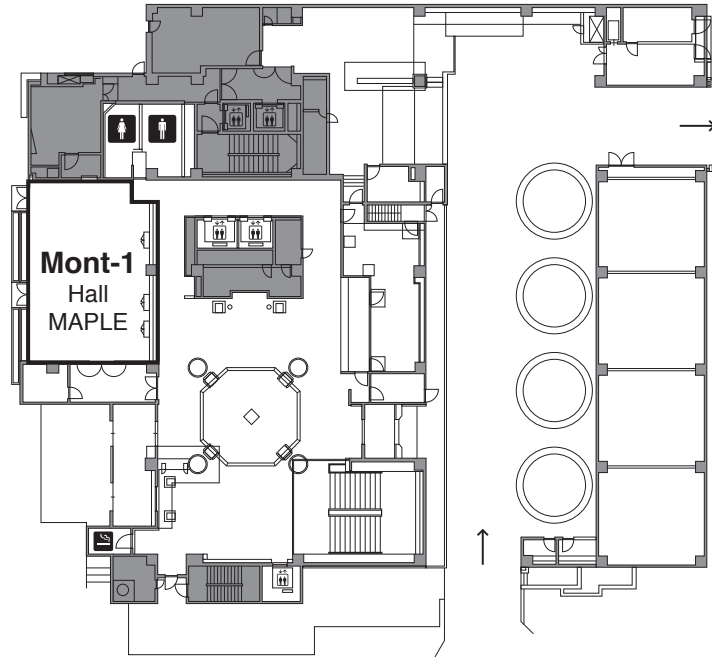
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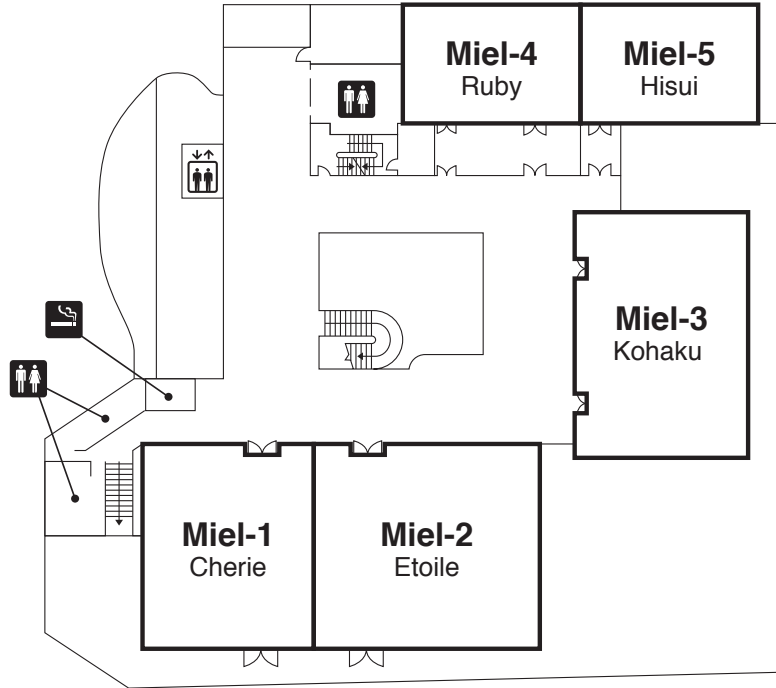


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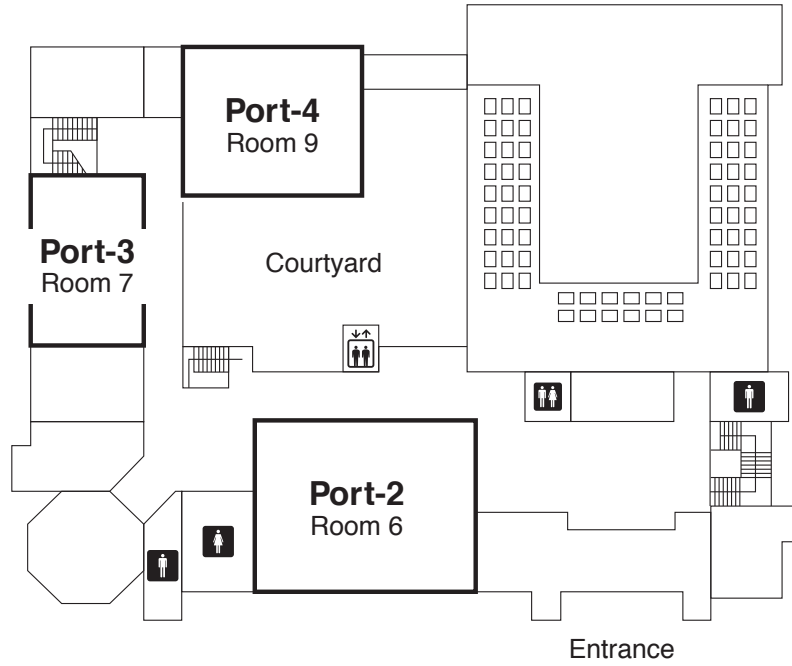
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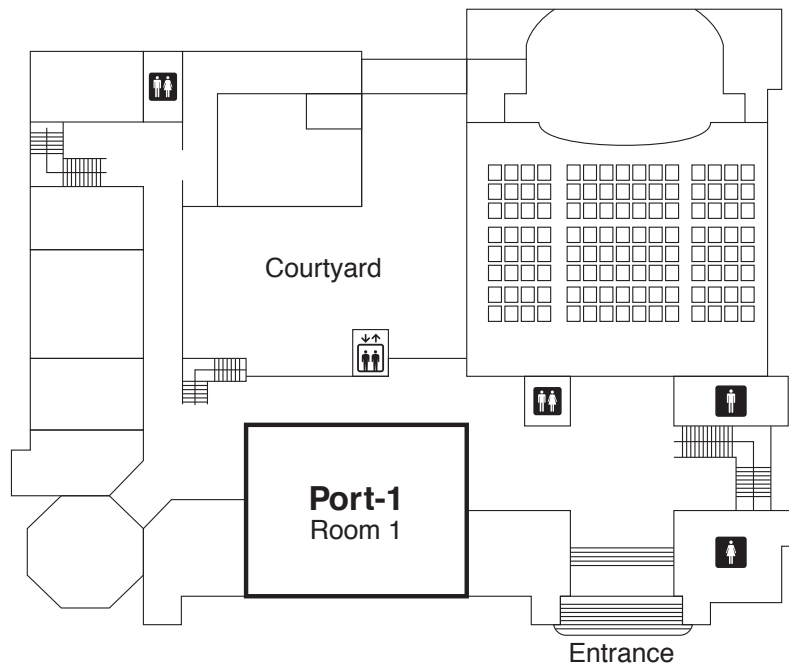


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Plenary Lectures

- PL-1** Experimental Modelling of Catalyst Materials at the Atomic Scale
- PL-2** Materials science for better batteries Achievements and future trends
- PL-3** $(\text{Al,Ga})_2\text{O}_3$ and $(\text{In,Ga})_2\text{O}_3$ Alloy Semiconductors in Various Crystal Phases: Physical Properties, Pseudomorphic Epitaxy and Device Perspectives
- PL-4** First-Principles Material Simulation and Beyond
- PL-5** High-entropy alloys
- PL-6** The Terrawatt Opportunity: new materials paradigms toward sustainability
- PL-7** Magnetic Materials: Innovation and Sustainable Development

December 10–13, 2019

Plenary Lectures

December 10, 2019

Opening Session 1-4

Opening
Hideo Hosono
 Tokyo. Tech. / Chairperson of MRM2019
 14:50–15:00

PL-1 15:00–15:40

Experimental Modelling of Catalyst Materials at the Atomic Scale

Hans-Joachim Freund
 Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany
 Chairperson: Tsunehiro Tanaka
 (Kyoto University)

PL-2 15:50–16:30

Materials Science for Better Batteries Achievements and Future Trends

Jean-Marie Tarascon
 College de France, France
 Chairperson: Atsuo Yamada
 (The University of Tokyo)

PL-3 16:40–17:20

(Al,Ga)₂O₃ and (In,Ga)₂O₃ Alloy Semiconductors in Various Crystal Phases: Physical Properties, Pseudomorphic Epitaxy and Device Perspectives

Marius Grundman
 Universitat Leipzig Institut für Experimentelle Physik,
 Germany
 Chairperson: Yuzo SHIGESATO
 (Aoyama Gakuin University)

PL-4 17:30–18:20

First-Principles Material Simulation and Beyond

Shinji Tsuneyuki
 The University of Tokyo, Japan
 Chairperson: Hidetoshi FUKUYAMA
 (Tokyo University of Science)

December 11, 2019

Session 5

PL-5 13:00–13:40

High-Entropy Alloys

Easo P George
 Oak Ridge National Laboratory and the University of
 Tennessee, USA
 Chairperson: Isao Tanaka
 (Kyoto University)

December 12, 2019

Session 6

PL-6 13:00–13:40

The Terrawatt Opportunity: New Materials Paradigms Toward Sustainability

David S. Ginley
 NREL Fellow, USA
 Chairperson: Hideo Hosono
 (Tokyo Institute of Technology)

December 13, 2019

Session 7

PL-7 13:00–13:40

Magnetic Materials: Innovation and Sustainable Development

Michael Coey
 Trinity College Dublin, Ireland
 Chairperson: Hisazumi Akai
 (The University of Tokyo)

PL-1

Experimental Modelling of Catalyst Materials at the Atomic Scale

Hans-Joachim Freund

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany

Hans-Joachim Freund is a scientific member and director at the Fritz-Haber-Institut der Max-Planck-Gesellschaft in Berlin where he is head of the Department of Chemical Physics. The department is dedicated to the study of model catalysts, applying a large number of techniques and instruments, some of which were newly developed within the department to investigate oxide surfaces and oxide metal interfaces. He serves as Adjunct Professor at five universities in Germany and UK. He received awards in Europe, the US, and Asia. He is a member of six Academies including the German National Academy of Sciences Leopoldi-na and the American Academy of Arts and Sciences and holds three honorary Doctorates. He received the Gaede-Langmuir Award of the American Vacuum Society and is the recipient of the 2015 Michel Boudart for the Advancement of Catalysis by the North American Catalysis Society and the European Federation of Catalysis Societies. He is Fellow of the American Physical Society and has published more than 815 scientific papers with more than 45.000 citations and given about 770 invited talks. He has held a number of named lectureships around the world. He has educated more than 130 PhD students and collaborated with more than 80 postdoctoral associates.



PL-2

Materials science for better batteries Achievements and future trends

Jean-Marie Tarascon

College de France, France

Jean-Marie Tarascon (1953) is Professor at the College de France holding the chair “Chemistry of solids – Energy). But much of his early career was spent in the United States where he discovered new electrolytes for Li-ion developed (1994) the plastic Li-ion technology. Back to France in 1995, he created the European network of excellence ALISTORE-ERI and more recently the French network on electrochemical energy storage (RS2E). Tarascon’s present research is devoted to batteries with emphasis on designing new materials and electrolytes, developing new eco-efficient synthesis processes, understanding reaction mechanisms, identifying novel reactivity concepts, and exploring chemistries beyond Li. .. He is the author of more than 650 scientific papers, and detains ~100 patents. He received many honours, with the last ones in 2017 being the CNRS innovation medal, the Galvani medal and the Eric and Sheila Samson Prime Minister’s Prize.



PL-3

(Al,Ga)₂O₃ and (In,Ga)₂O₃ Alloy Semiconductors in Various Crystal Phases: Physical Properties, Pseudomorphic Epitaxy and Device Perspectives

Marius Grundman

Universität Leipzig Institut für Experimentelle Physik, Germany

Marius Grundmann received his PhD (Dr. rer. nat., 1991) from Technische Universität Berlin (TUB). In 1992 he worked as post-doc at Bellcore, Red Bank, NJ, on quantum wires, then at TUB on self-organized semiconductor III-V quantum dots and devices based on them. Since 2000 he is professor for semiconductor physics at Universität Leipzig. His research interest is focused on oxide semiconductors in the form of bulk, thin films, heterostructures, microcavities and nanostructures for the use in transparent electronic devices and nanosystems. Among his most recent scientific achievements are the first general model for Raman scattering in anisotropic crystals, exceptional points in anisotropic micro-cavities and devices from amorphous zinc-tin-oxide and (p-type) copper iodide. He has published three books and over 550 journal papers with an h-index of 64 (WoS). He is a member of DPG, MRS, APS and Sächsische Akademie der Wissenschaften zu Leipzig. He currently serves as Director of the Felix Bloch Institute for Solid State Physics of Universität Leipzig.



PL-4**First-Principles Material Simulation and Beyond**

Shinji Tsuneyuki

University of Tokyo, Japan

Shinji TSUNEYUKI is a Professor in the Department of Physics, School of Science, The University of Tokyo from 2007. He received Ph. D on Physics at The University of Tokyo in 1990. His current research interest is in developing and applying methods of computational physics to clarify the physics of materials, to predict material properties, and to create new materials. Areas of current research include the transcorrelated method, a first-principles wave function theory for condensed matter; electronic properties and structural transformation of materials under high pressure; thermal properties of materials; quantum effect of light particles (protons, muons, etc.) in solids; impurities in ferroelectric materials; microscopic understanding of laser ablation; data assimilation and structure prediction of crystals. He won the IBM Japan Science Prize in Physics in 2001.

Since 2010, he has been working for the application software development project for the K computer and the post-K computer as a representative of the field of device and materials science.



1987-1992	Research Associate, Department of Physics, The University of Tokyo, Japan
1992-2002	Associate Professor, The Institute for Solid State Physics, The University of Tokyo
2002-2007	Associate Professor, Department of Physics, School of Science, The University of Tokyo, Japan
2007-present	Professor, Department of Physics, School of Science, The University of Tokyo, Japan Concurrent Professor, The Institute for Solid State Physics, The University of Tokyo, Japan
2011-present	Manager of the Center of Computational Materials Science, The Institute for Solid State Physics, The University of Tokyo, Japan

Current Research: Condensed Matter Physics Theory, Computational Materials Science

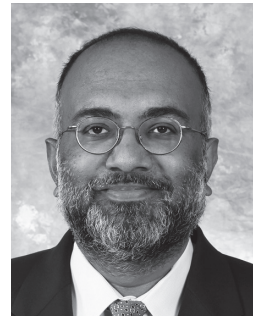
PL-5**High-entropy alloys**

Easo P George

Oak Ridge National Laboratory and the University of Tennessee, USA

Position: Governor's Chair for Advanced Alloy Theory and Development

Brief bio: Prior to taking up his current position, George was Professor of Materials Design and Director of the Center for Interface Dominated High Performance Materials at the Ruhr University Bochum in Germany. Before that, he was a distinguished research staff member at ORNL where he led the Alloy Behavior and Design Group and was a joint faculty professor of materials science and engineering at UT. George earned his PhD in materials science and engineering from the University of Pennsylvania, Philadelphia and BTech in metallurgical engineering from the Indian Institute of Technology, Kanpur. His current research interests include the physical metallurgy and mechanical properties of high-entropy alloys for structural applications, iridium and other refractory metals for space power applications, and size effects on mechanical behavior.



PL-6

The Terrawatt Opportunity: new materials paradigms toward sustainability

David S. Ginley
NREL Fellow, USA

Dr. David S. Ginley is currently Chief Scientist for Materials and Chemistry Science and Technology and a Research Fellow at the National Renewable Energy Laboratory. He received his PhD in Inorganic Chemistry from MIT and his BS in Chemistry from the Colorado School of Mines. He directed the Solar Energy Center for India and the US (SERIUS) and is chief experimentalist for the EFRC Center for Next Generation Materials by Design. Current work focuses on advancing solar and geothermal energy conversion and storage specifically in the areas of development and application of new materials by computational materials design in the areas of transparent conducting oxides, organic electronics materials, nano-materials and the development of process technology for materials and device development including; combinatorial methods, direct write materials, composite materials and non-vacuum processing for materials in extreme environments. A key focus is looking at how to significantly reduce the cost of renewable generated energy through novel devices and processing. He has over 400 publications and 40 patents.



PL-7

Magnetic Materials: Innovation and Sustainable Development

Michael Coey
Trinity College Dublin, Ireland

Michael Coey is Professor Emeritus at Trinity College Dublin, Ireland, and author of several books and many papers on magnetism and magnetic materials. These include contributions to amorphous and disordered magnetic materials, permanent magnetism, magnetism of soils and minerals, dilute oxides and magneto-electrochemistry, with more recent work on magneto-microfluidics, spin electronics, d-zero magnetism and half metals. A Fellow of the Royal Society and Foreign Associate of the National Academy of Science, he has served as Chairman of the IUPAP Magnetism Commission, and Divisional Associate Editor of Physical Review Letters. He founded Magnetic Solutions Ltd and the Trinity College Science Gallery, and was a promoter of CRANN, Ireland's nanoscience research centre. He was awarded the 2019 Max Born Medal by the German Physical Society.



PL-1

Experimental Modelling of Catalyst Materials at the Atomic Scale

Hans-Joachim Freund¹¹ Fritz Haber Institute of the Max Planck Society, Berlin, 14195, Germany, freund@fhi-berlin.mpg.de

Keywords: Model Catalysts, Strong Metal-Supported Interaction, Confined Space, Reaction at Metal-Oxide Interface,

In order to capture the complexity of real powder catalysts, we have tried to develop an approach that adds complexity in a controlled way starting from simple model systems. The experimental techniques come from the tool box of surface science. We will discuss a number of systems addressing different questions, including:

- Which role is played by the metal oxide interface in a chemical reaction involving charge transfer? (Fig.1)¹
- What is the role of the Strong Metal Support Interaction (SMSI) of supported catalysts in a simple oxidation reaction such as CO oxidation?²
- Is it possible to use surface science approaches to learn something about confined space reactions? (Fig.2)³

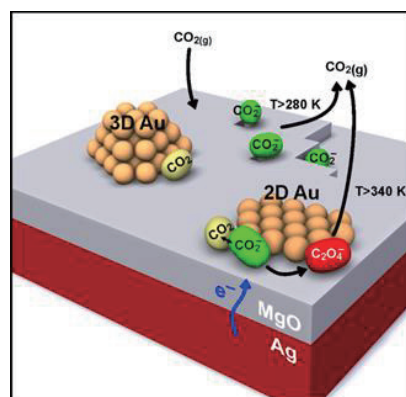


Fig. 1. Thin film MgO/Ag system controlling the morphology and electron charge transfer of supported Au nano-particles in CO₂ activation

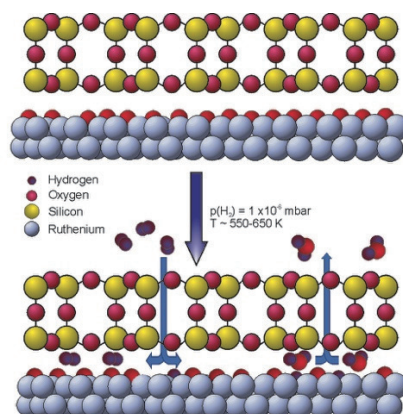


Fig. 2. Water formation in confined space between a crystalline/vitreous silica film and a Ru(1000) surface in direct comparison to the open space reaction.

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PL-2

Materials science for better batteries Achievements and future trends

Jean-Marie Tarascon

Collège de France, - UMR CNRS 8260, 11 Place Marcelin Berthelot, 75005 Paris, France
Réseau sur le Stockage Electrochimique de l'Energie (RS2E) - FR CNRS 3459, 80039 Amiens Cedex,
France

jean-marie.tarascon@college-de-france.frabc@defg.hij.ac.jp

Li-ion, Na-ion, batteries, anionic-redox, sensing

Research's progresses in rechargeable batteries are driven by ever increasing demands for portable electronic devices as well as for powering electric vehicles and providing load-leveling for mass storage of renewable energy. Li-ion batteries are the systems of choice for the aforementioned applications. Therefore, for this to fully happen, new concepts and new sustainable chemistries are sorely needed, and this is what this presentation will address.

Firstly, regarding new concepts, we will show how the discovery of a new Li reaction mechanism that involves the anionic network with the reversible formation of dimers (O-O) represents a transformational approach for creating electrode materials with exacerbated capacities⁽¹⁾. Towards, higher energy density systems, recent advances on solid state Li batteries will be discussed. Concerning new chemistry, we will present our new findings with the Na-ion chemistry which enlists novel materials/electrolyte designs⁽²⁾ and the assembly of practical 18650 prototypes prior to touch on our recent studies with aqueous systems. Lastly, an indirect way to enhance simultaneously energy density and sustainability via the use of sensing and self-healing functionalities will be introduced. Through these examples, we hope to convey that the future of battery offers new opportunities for materials scientists as long as we are willing to explore new risky paths.

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PL-3

(Al,Ga)₂O₃ and (In,Ga)₂O₃ Alloy Semiconductors in Various Crystal Phases: Physical Properties, Pseudomorphic Epitaxy and Device Perspectives

Marius Grundmann¹¹ Universität Leipzig, Felix Bloch Institute for Solid State Physics, Leipzig, 04105, Germany grundmann@physik.uni-leipzig.de

Keywords: Oxide Semiconductors, Sesquioxides, Gallium Oxide, Heterostructures

The binary sesquioxide semiconductor Ga₂O₃ and related materials have been in research focus for a few years due to its possible use in high power transistor applications [1]. Electromobility and renewable energies drive the demand for devices that can surpass the performance of SiC or GaN. Epitaxial layers of this material have been realized by us in various phases using physical [2] and chemical [3] methods. Other devices such as (deep) UV photodetectors, transparent inter-subband detectors and HEMT can be envisioned from heterostructures employing (In,Ga)₂O₃ or (Al,Ga)₂O₃ alloy layers. Especially interesting for HEMT's is the κ-phase, exhibiting possibly a large spontaneous polarization and high electron interface density (2DEG).

Similar to the situation in arsenide and nitride alloy semiconductors, the oxide sesquioxide alloys exhibit an increase (decrease) of lattice constant with indium (aluminum) incorporation. Using combinatorial epitaxial techniques (Fig. 1), we have determined the phases and their alloy concentration ranges and their dependence on growth parameters. The stress-strain relation of pseudomorphic layers on lattice-mismatched substrates has been modeled by us in the framework of continuum elastic theory for various phases, in particular the monoclinic (β), orthorhombic (κ) and trigonal (corundum) (α) phases [4,5].

The oxide alloy semiconductors exhibit a decrease (increase) of their band gap energy with indium (aluminum) incorporation. We have investigated this effect in detail using spectroscopic ellipsometry. The optically anisotropic character of the materials (birefringence and dichroism) is discussed in detail [6]. The consequences for correct evaluation of Raman scattering are pointed out [7]. Also, the band alignment with different dielectrics is discussed.

This work has been done in cooperation with H. von Wenckstern, M. Lorenz, M. Kneiß, D. Splith, A. Hassa, C. Sturm, T. Schultz, N. Koch, M. Albrecht, Ch. Fares, S.J. Pearton, members of the GraFOx consortium and others. Parts of this work have been funded by European Social Fund within the Young Investigator Group "Oxide Heterostructures" (SAB 100310460) and by Deutsche Forschungsgemeinschaft in the framework of Sonderforschungsbereich 762 "Functionality of Oxide Interfaces" (projects A02, B04).

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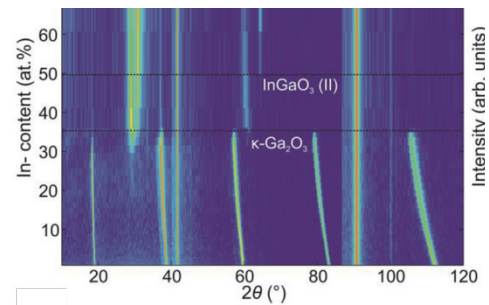


Fig. 1. False color image of 55 XRD 2θ-ω measurements of (In,Ga)₂O₃ layer, acquired along the gradient direction of a PLD combinatorial epitaxy wafer. Up to an In-content of 35 at.%, the κ-phase exists.

PL-4

First-Principles Material Simulation and Beyond

*Shinji Tsuneyuki^{1,2}

¹ Department of Physics, School of Science, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan, ² Institute for Solid State Physics, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, Japan.

* stsune@phys.s.u-tokyo.ac.jp

Keywords: Computer simulation, first-principles calculation, data centric science,

Material simulation based on the first-principles calculation of electronic states aims to explain the physics of materials, to predict material properties, and to create new materials by fully utilizing high-performance computers. In line with the development of computer hardware, novel computational methods and algorithms have been developed for such purposes, and they are opening new doorways in materials science and technology with connecting theories and experiments.

In this presentation, I will give a brief overview of recent advances and remaining problems in the first-principles simulation from the viewpoint of accuracy, system size, dynamics, and exploration. I will show that some of these problems are solvable by a combination of first-principles calculation with modeling and data-centric science approaches.

The first example is the simulation of the thermal properties of crystals, where a precise calculation of the anharmonic phonon effect is necessary. Although the spatiotemporal scale of phonon properties is so diverse, the thermal properties and their temperature dependence can be precisely calculated by a combination of first-principles molecular dynamics and so-called sparse modeling^{1,2}.

The second one is the theoretical exploration of crystal structures. There has been much progress in the methodology of crystal structure prediction for years, and yet it is a severe problem if the number of atoms exceeds ~50. Here I will show that crystal structure exploration is efficiently accelerated by the Bayes' theorem with a little help from incomplete powder-diffraction data^{3,4}. The method is helpful for high-pressure materials science.

The third example is the simulation of non-thermal laser ablation by a femtosecond laser pulse. First-principles calculation of a small and idealized system has brought an idea for the mechanism of this complex phenomenon, while model simulations with first-principles parameters have given strong support by comparison with experimental data⁵.

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PL-5

High-entropy alloys

E. P. George^{1,2}¹ Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831-6115, USA² Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN, 37996-2100, USA georgeep@ornl.gov

Keywords: Structural materials, Mechanical properties, Microstructure, Deformation mechanisms

Conventional alloys consist of a primary element chosen with a primary property in mind (e.g. gold for luster) to which secondary elements are added for other properties (e.g. copper for strength). Recently, however, a novel alloy design strategy has taken the metallurgical world by storm, as summarized in a recent review [1]. It eschews the primary-element approach and, instead, mixes together four, five, or more elements in near-equal amounts. These alloys have high (ideal) entropies of mixing – hence the name. They are scientifically interesting because theories that have been developed for dilute solid solutions break down in concentrated alloys lacking “solvents” or “solutes” in the traditional sense. A handful also exhibit striking mechanical properties (Fig. 1), including strength [2,3], ductility [2,3], and toughness [4,5] that are simultaneously enhanced at cryogenic temperatures, unlike in conventional materials where they have to be traded off.

The multidimensional compositional space occupied by high-entropy alloys remains largely unexplored. One of the reasons for the current excitement in the field is that many more alloys may be lurking in these regions, just waiting to be discovered. A possible strategy for narrowing down the search area relies on identifying both the physical mechanisms responsible for the superior properties as well as their composition dependence. Such a bottom-up approach allows a more targeted probing of limited areas within the available composition space. In this talk, I will summarize what we have learned about the mechanical properties of this new class of alloys. By focusing on a few model systems, it is possible to gain fundamental mechanistic understanding of certain properties and phenomena. These insights serve as a useful guide to navigate the vast multi-dimensional space that remains to be explored. They also help us develop broadly applicable scientific principles for alloy design.

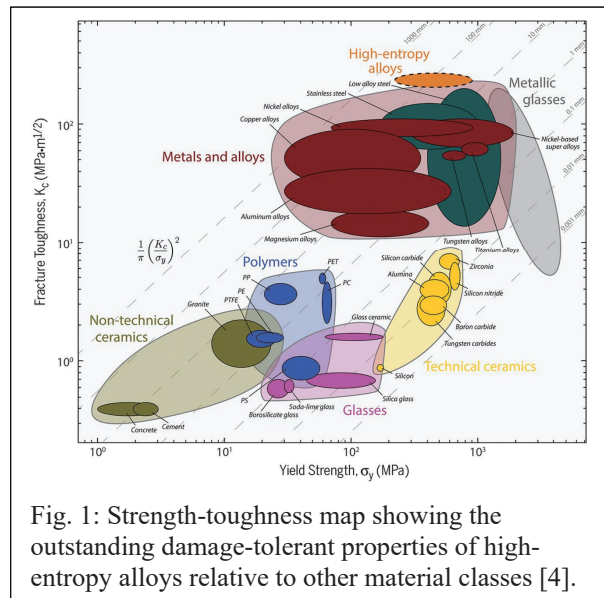


Fig. 1: Strength-toughness map showing the outstanding damage-tolerant properties of high-entropy alloys relative to other material classes [4].

References:

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PL-6

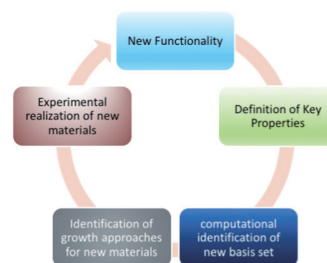
The Terrawatt Opportunity: new materials paradigms toward sustainability

David Ginley, Kristin Persson², Lauren Garten¹, Praneetha Selvarasu¹, John Perkins¹, Wenhao Sun², Kirill Popov², Shyam Dwaraknath², Gerbrand Ceder², John Mangum³, Brian Gorman³, Laura Schelhas⁴, Michael Toney⁴, Zamyra Chan⁵, Daniel Nocera⁵, James Haggerty⁶, Okan Agirseven⁶, Janet Tate⁶, Daniil Kitchaev⁷, Nancy Haegle¹, William Tumas¹

¹NREL; ²Lawrence Berkeley National Laboratory; ³Colorado School of Mines; ⁴SLAC National Accelerator Laboratory; ⁵Harvard University; ⁶Oregon State University; ⁷Massachusetts Institute of Technology

There is an increasing realization that long term sustainability requires significant societal changes from both in infrastructure and in use patterns. This requires significant restructuring of our overall energy systems including an increasing integration of renewable energy generation with active storage, a minimization of CO₂ generating energy technologies and transformations in transportation and buildings. To achieve the kind of penetration of renewable energy needed is both a challenge and an opportunity. Si solar cells are headed toward being the largest business on the planet. To achieve such a large shift in the topology of our energy systems requires new functional materials and just as importantly approaches on how to make them. We can no longer afford the 20 year cycle from discovery to application in a new material or device.

We view the approach as being similar to that shown in the figure, whereby the desired functionality is defined as are the key properties needed for an applications space; such as temperature, chemical environment etc. Computationally this can lead to a definition of a set of potential materials and then upon down selection of appropriate candidates it is possible to computationally examine a number of synthetic pathways including possible substrate and or approaches to nucleation and growth. We will demonstrate this approach with examples of the targeted synthesis of high energy polymorphs of SrHfO₂ that are piezoelectric (the ground state is not). And by targeted solution synthesis of polymorphs of MnO₂ and TiO₂ with diverse functionality. This new methodology for the realization of new functional and metastable materials is foundational toward developing a sustainable society.



This work was supported by the US Department of Energy, Office of Science, Office of Basic Energy Sciences, as part of the CNMGE Energy Frontier Research Center under contract No. DE-AC36-08GO28308 to NREL.

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Dr. David Ginley, Research Fellow/ Chief Scientist
Materials and Chemistry Science and Technology
NREL
15313 Denver West Pkwy
Golden, CO 80401
303-384-6573ph, 303-384-6430 fax
720-375-4240 cell
David.ginley@nrel.gov

PL-7

Magnetic Materials: Innovation and Sustainable Development.

J. M. D. Coey, School of Physics and CRANN,
Trinity College Dublin, Ireland.

Magnetic materials are important in a huge range of applications; two principal categories are bulk functional materials and thin films for data recording and electronic devices. An increasing focus on energy efficiency and sustainability is driving a quest for new materials and reshaping how we think about existing solutions. *Soft magnets* are already highly efficient and barring a breakthrough on the Slater Pauling curve, scope for improvement is limited. *Permanent magnets* create a magnetic field in their surrounding space with no continual expenditure of energy. An electromagnet producing 1 Tesla in a volume of 500 cc will consume \$2000 worth of energy over 10 years. A permanent magnet does the same job for free. Although the energy stored in the magnetic field is only 200 Joules — it is in a particularly useful form, providing the basis of highly-efficient energy converters, both electric motors and generators. Demand for rare-earth magnets for new applications, notably electric vehicles and robotics, but also direct-drive wind turbines and microscale energy harvesting, is increasing rapidly from the present base of 100,000 tonnes per annum. The 2011 rare earth crisis focussed attention worldwide on reducing and recycling heavy rare earths.

Regarding archival recording, a focus is on developing media structures compatible with heat-assisted *magnetic recording*. As digital data processing consumes ever-greater quantities of energy the challenge to magnetic or other solutions is to drastically curb the energy requirement to sustain information technology and to advance data rates into the terahertz gap, where chip-based *spin electronics* solutions could be attractive.

Finally, there are prospects of magnetic materials based on entirely new principles, that will be discussed briefly.

Cluster Keynotes

Ken-1

- A. Fundamentals for Materials**
- B. New Trend of Materials Research**
- C. Novel Structural Materials Based on New Principles**
- D. Advanced Electronic Materials**
- E. Magnet and Spintronics**
- F. Energy**
- G. Materials for Smart Systems**
- H. Green Technology and Processing**
- I. Biopolymers**

December 10–13, 2019

Cluster Keynotes

Ken-1

December 11, 2019

Cluster Session A

Time 16:30–18:30

Chairpersons Shin-ichi ORIMO, Koichi HAYASHI,
Taisuke OZAKI

AX-11-CLK01 16:30–17:10

Ions and electrons at interfaces of functional ionic materials

Truls NORBY
University of Oslo, Norway

AX-11-CLK02 17:10–17:50

White Neutron Holography – New Probe of Local Atomic Structures around Dopants in J-PARC

Kenji OHYAMA
Ibaraki University, Japan

AX-11-CLK03 17:50–18:30

Bridging atomic-resolution experiment and computation using machine learning

Teruyasu MIZOGUCHI
The University of Tokyo, Japan

December 12, 2019

Cluster Session B

Time 9:30–12:00

Chairperson Shinji Tsuneyuki

BX-12-CLK01 9:30–10:20

When the New Science is in the Outliers

Matthias Scheffler
Fritz Haber Institute of the Max Planck Society, Germany

BX-12-CLK02 10:20–11:10

Data driven discovery of new materials

Isao Tanaka
Kyoto University, Japan

BX-12-CLK03 11:10–12:00

Geometric frustration and the intrinsic approach in material science

Efi Efrati
Weizmann Institute of Science, Israel

December 13, 2019

Cluster Session C

Time 14:00–16:00

Chairpersons Eiji Abe, Junichi Tatami, Kozo Ito

CX-13-CLK01 14:00–14:40

Evolution of LPSO Structure to Mille-Feuille Structure in Ultrahigh-Strength Magnesium Alloys

Yoshihito KAWAMURA
Kumamoto University, Japan

CX-13-CLK02 14:40–15:20

Additive Manufacturing of Ceramic Components with Unique Structures

Tatsuki OHJI
National Institute of Advanced Industrial Science and Technology, Japan

CX-13-CLK03 15:20–16:00

Detecting bond scission in fracture of soft materials

Prof. Costantino Creton
CNRS Research Director, ESPCI, Paris Tech, France

December 12, 2019

Cluster Session D

Time 14:00–16:00

Chairpersons Yoshihiro Iwasa, Kenji Shiojima, Susumu Saito

DX-12-CLK01 14:00–14:40

Atomic-level control of high temperature superconductor materials for unveiling their pairing mechanism

Qi-kun XUE
Tsinghua University, China

DX-12-CLK02 14:40–15:20

Development of Corundum-Structured Gallium Oxide Power Devices by MIST EPITAXY®

Takashi SHINOHE
FLOSFIA INC., Japan.

DX-12-CLK03 15:20–16:00

Emergent electromagnetism in quantum materials

Naoto NAGAOSA
RIKEN and U. Tokyo, Japan

December 11, 2019

Cluster Session E

Time 9:30–12:05

Chairpersons YoshiChika Otani, Jun Sugiyama

EX-11-CLK01 9:30–10:10

Antiferromagnets for neuromorphics and opto-electronics

Tomas Jungwirth

University of Nottingham/Institute of Physics, Academy of Sciences of the Czech Republic, United Kingdom

EX-11-CLK02 10:10–10:50

Quantum Criticality in Organometallics Studied by Neutrons & Muons

Martin Månsson

Royal Institute of Technology, Sweden

 Break
10:50-11:05

EX-11-CLI03 11:05–11:35

Probing antiferromagnets with currents

Vincent Baltz

SPINTEC - Univ. Grenoble Alpes / CNRS / CEA / GINP, France

EX-11-CLI04 11:35–12:05

Nanocrystalline formation of the iron based soft magnet FINEMET studied by operando muon spin rotation technique

Akihiro Koda

KEK IMSS, Japan

December 12, 2019

Cluster Session F

Time 16:30–18:30

Chairpersons Yoshiharu SAKURAI, Atsuo YAMADA, Takao MORI

FX-12-CLK01 16:30–17:10

Hard X-ray spectro-ptychography: Visualization of heterogeneous oxygen storage behavior in three-way catalyst particles

Yukio TAKAHASHI

Osaka University, Japan

FX-12-CLK02 17:10–17:50

Quantifying Inactive Lithium in Lithium Metal Batteries

Ying Shirley MENG

University of California San Diego, USA

FX-12-CLK03

17:50–18:30

Withdrawal

December 13, 2019

Cluster Session G

Time 9:30–11:50

Chairperson Tsutomu Miyasaka

GX-13-CLK01

9:30–10:05

Soft Electronic and Robotic Systems

Martin Kaltenbrunner

Johannes Kepler University Linz, Austria

GX-13-CLK02

10:05–10:40

Design, development, and doping of novel inorganic optoelectronic functional materials

Toshio Kamiya

Tokyo Institute of Technology, Japan

GX-13-CLK03

10:40–11:15

Gold Nanorods with Ultranarrow LSPR Bands

Luis M. Liz-Marzán

CIC biomaGUNE, Spain

GX-13-CLK04

11:15–11:50

Perovskite Solar Cells: History, Progress and Perspective

NamGyu Park

School of Chemical Engineering, Sungkyunkwan University, Korea

December 11, 2019

Cluster Session H

Time 14:00–16:00

Chairpersons Katsuya Teshima, Tetsuya Yamamoto

HX-11-CLK01

14:00–14:30

Photocatalytic water splitting for solar hydrogen production

Kazunari Domen

The University of Tokyo / Shinshu University, Japan

HX-11-CLK02

14:30–15:00

Plasma Synthesis, Conversion, and Processing of Energetic Materials

Alexander Fridman

Drexel University, USA

HX-11-CLK03

15:00–15:30

Gallia(Ga₂O₃) for Green and Efficient Energy applications

Ekaterina Chikoidze

Paris Saclay University, France

HX-11-CLK04

15:30–16:00

Lead-free Piezoelectric Ceramics – Future perspectives –
Akira Ando
Murata Manufacturing Co., Ltd., Japan

December 13, 2019

Cluster Session I

Time 16:30–18:00

Chairpersons Jun Kikuchi, Masaya Yamamoto

IX-13-CLK01

16:30–17:15

Importance of strengthening “venous industry” for future plastics
Nobuyuki Kawashima
Mitsui Chemicals, Inc., Japan

IX-13-CLK02

17:15–18:00

Ceramic Additive Manufacturing Technologies for Biomedical applications
Hui-suk Yun
Korea Institute of Materials Science, Korea

AX-11-CLK01

Ions and electrons at interfaces of functional ionic materials

*Truls Norby¹

¹Dept. Chemistry, Centre for Materials Science and Nanotechnology, Univ. of Oslo, NO-0318 Oslo, Norway

* truls.norby@kjemi.uio.no

Keywords: Grain boundaries; heterointerfaces; surfaces; protons; electrons

The thermodynamics and kinetics of ionic and electronic defects in the bulk of crystalline ionic materials describe well the equilibrium deviation from the perfect structure as well as random and gradient-driven transport. Once heterogeneities like homo- or heterojunctions or surfaces are introduced, defect energies vary spatially, introducing primary equilibrium concentration gradients and charge separation, as well as secondary space charge regions with depletion or enrichment of charge carriers, causing large variations in transport properties. Examples comprise the highly resistive grain boundaries of oxide and proton conducting ceramics, the job-sharing separation of charged ionic defects and electronic species over heterointerfaces, and surface protonic conduction in adsorbed water. In this talk I discuss some of these aspects in further detail.

The high resistance of grain boundaries in acceptor-doped oxide ion and proton conducting ceramics is assigned to depletion of positive charge carrying defects in the space charge layers, caused by the accumulation of the same carriers in the core of the grain boundary for relaxation of lattice mismatch strain. But the positive charge of the core is hard to vary directly. We have applied TEM electron holography to a grain boundary in Y-doped BaZrO₃.¹ This yields a phase shift of the electron beam caused by the local charge through the sample. Surprisingly, the grain boundary core appears negative rather than the expected positive. This can to some extent be understood by the loss of Ba²⁺ by out-diffusion to evaporation and formation of surface carbonate, competing with the accumulation of effectively positive oxygen vacancies and protons. But more importantly, the high energy TEM electrons used in holography feel a different local electrical potential – dominated by the spatial function of the positive atomic nuclei - than the comparatively stationary protons – dominated by the orbitals of the negative electron clouds.

As another example, I discuss recent computational results² on the heterointerface between two undoped ionic materials – BaZrO₃ and SrTiO₃ – showing how different defect formation energies can form charge separation between the two materials close to the interfaces, leaving one with effectively positive ionic defects and the other with charge compensating negative defects, e.g. electrons. This may lead to development of for instance mixed ion-electron conducting (MIEC) nanocomposites with charge carriers with high mobilities due to the lack of trapping to heterovalent dopants. The heterointerface effectively induces a doping effect in both materials.

Finally, I discuss new directions in surface protonics. There is growing understanding and parameterisation of the fundamentals of conduction of free protons in chemisorbed and ice-like physisorbed water, and of vehicular protonic species in thicker liquid-like physisorbed water layers at high relative humidities.³ This is caused by charge separation between the surface and the water and has large effects on a range of physicochemical processes e.g. on surfaces of catalysts and in nanoporous ceramics. But recent advances in heterogeneous catalysis enhanced by surface protonic currents on ceramic supports in the presence of dry hydrogen (no water)⁴ requires new insight in dissociation and ionisation of hydrogen on ionic surfaces.

References:

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- 4) R. Manabe, S. Okada, R. Inagaki, K. Oshima, S. Ogo, Y. Sekine, *Scientific Reports*, [6] (2016) 38007.

Truls Norby

Professor, University of Oslo

Truls Norby (b. 1955) has his PhD from the University of Oslo (UiO) 1986, where he studied and worked with late prof. Per Kofstad.

Norby became professor at the Department of Chemistry 1994 and head of the Group for Solid-State Electrochemistry in 1997, now Group for Electrochemistry, which is part of the Centre for Materials Science and Nanotechnology (SMN) at UiO.

Norby works with thermodynamics and transport of defects in materials for solid-state fuel cells, electrolyzers, batteries, gas separation membranes, sensors, and metal protection oxide layers. He specialises in protons in oxides and their use in high temperature proton conductors and hydrogen separation membranes. Recently, he also focuses on topics related to transport in adsorbed layers on surfaces and across interfaces (grain boundaries, electrodes) and on the semiconducting properties of oxides for uses in photoelectrochemistry and thermoelectrics.

He has published more than 240 journal papers, graduated 80 Master- and PhD-students, and is editor of Solid State Ionics and President of the International Society for Solid State Ionics (ISSE) 2019-2021. He is member of the Norwegian Academy of Science and Letters and other national academies. He has won the UiO Innovation Prize (2012) and the Norwegian Guldberg-Waage medal for chemistry 2018.

He has founded companies NORECS AS (2001) which develops, manufactures, and sells test equipment world-wide (including China) and Protia AS (now CoorsTek Membrane Sciences AS) (2007) which develops energy conversion processes using proton conducting ceramic materials.



AX-11-CLK02

White Neutron Holography – New Probe of Local Atomic Structures around Dopants in J-PARC

*Kenji Ohoyama

Ibaraki Univ., Tokai, Ibaraki 319-1106, Japan

* kenji.ohoyama.vs@vc.ibaraki.ac.jp

Keywords: local atomic structure, light elements, neutron holography, dopants

For most of functional materials, the properties can be controlled by impurity doping. For Si semiconductors, B or P with a concentration of 10^{-5} - 10^{-9} are doped to enhance transportation properties. Thus, the slightly distorted atomic structure around dopants, called “*local structure*”, must be important for the functionality. The most powerful probe for visualisation of local atomic structures is atomic resolution holography (ARH), which can visualise 3D atomic structures in the range of ~ 20 Å from the selected atoms (dopants). ARH has been already established using fluorescent x-rays, and photoelectrons.

However, light elements, such as H, Li or B, which are important for novel functional materials, cannot be observed by x-rays and electrons. To overcome this, neutron ARH, which have higher sensitivity to light elements, was proposed and developed by Cser *et al.* and Sur *et al.* in 2001 using a monochromatic beam¹⁾. Recently, our group has succeeded in enhancing accuracy of atomic images drastically by using *white* neutrons in Japan Proton Accelerator Research Complex (J-PARC) at Tokai, Japan²⁾. Note that we can obtain data (holograms) with at most 130 wavelengths in the range of 0.36 – 6.5 Å at once; this is the essential point of the high accuracy. We successfully visualised local atomic structures around Eu in 1% Eu doped CaF₂, which is a typical scintillation crystal, and found that there exist excess F⁻ around Eu³⁺ dopants. We also succeeded in visualising local atomic structures in many materials: the semiconductor 0.26% B doped Si³⁾, the thermoelectric material 0.75% B doped Mg₂Si, the typical strongly correlated electrons system 2% Sm doped RB₆ (R: Yb, La), and so on. Fig.1 shows local structure around ¹⁰B (green) in 0.27 % ¹⁰B doped Si obtained by white neutron ARH in J-PARC³⁾. The Si structure around doped ¹⁰B is the diamond structure, directly indicating that most of ¹⁰B is located at Si positions. This indicates that the positions of light dopants can be determined by this method. Fig.2 shows atomic images of Yb around Sm (green) in 2% Sm doped Yb¹¹B₆ (space group:Pm-3m, *a* = 4.16 Å). We also visualised B cages around rare earth atoms. At least 7th nearest neighbour Yb located at 12.5 Å from Sm was visualised, which is much longer than the typical range of x-ray absorption fine structure method. Thus, one can observe change of doping effects to the atomic structures of light and heavy elements in the large area from the area around dopants to the area which has the non-distorted structure without doping effects.

By using the white neutron ARH, one can discuss doping effects (lattice distortions and/or fluctuations) by light element doping, such as B, or positions of light dopants, as well as local atomic structures of light elements around dopants. Thus, this technique is important to clarify the origins of properties in doped materials from a view point of structural physics.

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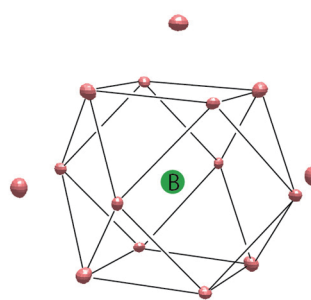


Fig. 1 Local structure of Si around ¹⁰B (green) in 0.27 % ¹⁰B doped Si obtained by white neutron ARH in J-PARC³⁾. Reproduced with permission.

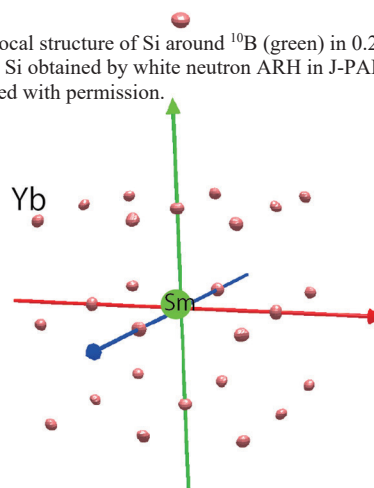


Fig. 2. Local structures of Yb around Sm (green) in 2% Sm doped Yb¹¹B₆. The distance between Yb is 4.16 Å

Kenji Ohoyama was born in Tokyo, Japan in 1961. He obtained his B.Sc.(1986) and M.Sc. (1988) degrees from Tohoku University, and Ph.D. from Tohoku University in 1992. He worked in Institute for Materials Reserch of Tohoku University as a research associate (1992–2003), associate professor (2003–2013), and as an associate professor in Advanced Institute for Materials Research of Tohoku University (2013-2015). He moved to Ibaraki University as a full professor in 2015. His main research fields are investigations of materials science and magnetism in strongly correlated electron systems using neutron scattering, and developing novel techqniues of neutron scattering.



AX-11-CLK03

Bridging atomic-resolution experiment and computation using machine learning

*[Teruyasu Mizoguchi](mailto:teru@iis.u-tokyo.ac.jp)¹, Shin Kiyohara¹, and Tomohiro Miyata^{1,2}

¹Institute of Industrial Science, University of Tokyo, Tokyo, 153-8505, Japan

²Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 2-1-1, Sendai, Japan

*teru@iis.u-tokyo.ac.jp

Keywords: Machine learning, spectroscopy, ELNES/XANES, first principles simulation, STEM

A combination between the experimental and computational investigations are crucial for the modern materials developments. In particular, an atomic scale investigation becomes more important for the recent down-sizing of the electric devices. On the other hand, one has to know that the “observation” is not identical to the “understanding”.

In recent years, machine learning approaches have widely spread in materials science to predict material properties quantitatively and overcome various obstacles with extensive computations. The machine learning was also applied to investigate lattice defects, such as grain boundary, and spectroscopic data, such as infrared (IR), nuclear magnetic resonance (NMR), ELNES/XANES, and extended X-ray absorption fine structure (EXAFS) to extract hidden information.

We are applying the machine learning method to build the bridge between the atomic resolution experiments and computations. In this presentation, I am going to present about following topics. 1) Atomic resolution analysis of liquid, 2) machine learning for ELNES/XANES. The respective contents are as blow:

1) Atomic resolution analysis using aberration-corrected STEM-EELS has been mainly applied to crystalline materials. On the other hand, its applications to liquid and gas have been limited. Recently, we are performing the atomic resolution analysis of ionic liquid [1-3] and investigation of the dynamic behavior of the gaseous molecule [4].

Ionic Liquids have characteristic properties, such as non-volatility, high ionic density, and hydrophilicity. Owing to such properties, ionic liquids have been studied for the wide range of applications. Atomic resolution observation of a gold doped ionic liquid was conducted by STEM-EELS. TEM specimen for the ionic liquid was fabricated using the simple method [1], and gold atoms were clearly observed as bright spots. We also observed the dynamics of monatomic ions in ionic liquids [2]. Quantitative molecular and ionic mapping in the ionic liquid was also achieved [3].

2) To develop a method that can interpret the ELNES/XANES spectra, hierarchical tree and decision tree methods are combined. First, ELNES/XANES database was constructed by the theoretical calculation. Then, hierarchical clustering was performed on the database, resulting in categorizing similar spectra into clusters. Spectral similarity was measured by cosine distance. Cutting the hierarchical tree at arbitrary threshold makes some clusters of the spectra. We successively lowered the cutting threshold to each branch point, resulting in making two clusters at every branch point. By using the branch point in the cluster as the teacher, the decision tree on the materials information was constructed by the supervised learning. We have confirmed that this method can correctly interpret the spectra [5].

In addition to the “interpret” the spectrum, the machine learning method was also applied to directly predict the materials structure and functions [6].

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- 6) S. Kiyohara et al., *J. Phys.: Materials*, 2 (2019) 024003-1-9



Teruyasu Mizoguchi is a professor in Institute of Industrial Science, The University of Tokyo. He received PhD from Kyoto University in 2002. From 2002~2005, he has been a postdoctoral researcher at Kyoto University, The University of Tokyo, and Lawrence Berkeley National Laboratory. He became a research assistant in Institute of Engineering Innovation, Graduate School of Engineering, The University of Tokyo in 2005 and an assistant professor in 2007. He moved to Institute of Industrial Science, The University of Tokyo in December 2009, as an associate professor and became a professor in January 2019. His research interest is investigating structure-property relationships of materials using atomic resolution electron microscopy and spectroscopy (STEM-EELS), first principles simulations, and machine learning.

BX-12-CLK01

When the New Science is in the Outliers

Matthias Scheffler^{1,2,}

¹ Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

² IRIS Adlershof, Humboldt-Universität zu Berlin, Zum Großen Windkanal 6, D-12489 Berlin, Germany

* Scheffler@fhi-berlin.mpg.de

Keywords: Big data, artificial intelligence, machine learning, compressed sensing, domain of applicability, materials science

Several issues hamper progress in data-driven materials science. In particular, these are a missing FAIR [1] data infrastructure and appropriate data-analytics methodology [2].

Significant efforts are still necessary to fully realize the A (accessibility) and I (interoperability) of FAIR. Here the development of metadata, their intricate relationships, and data ontology need more attention. Obviously, a FAIR data infrastructure – for being accepted by the community – should work without bureaucratic hurdles or the needs for special training. In this talk, I will discuss the challenges and progress, focusing on computational materials science.

Concerning the data-analytics, we note that the number of possible materials is practically infinite, but only 10 or 100 of them may be relevant for a certain science or engineering purpose. In simple words, in materials science and engineering, we are often looking for “needles in a hay stack”. Fitting or machine-learning all data (i.e. the hay) with a single, global model may average away the specialties of the interesting minority (i.e. the needles). I will discuss methods that identify statistically-exceptional subgroups in a large amount of data, and I will discuss how one can estimate the domains of applicability of machine-learning models.[3]

1) FAIR stands for Findable, Accessible, Interoperable and Re-usable. The FAIR Data Principles;
<https://www.force11.org/group/fairgroup/fairprinciples>

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Prof. Dr. Matthias Scheffler

Director at the Fritz Haber Institute (FHI) of the Max Planck Society (MPG), Berlin, Germany

Homepage: www.fhi-berlin.mpg.de/th/



Matthias Scheffler is known for his pioneering work linking density-functional theory with thermodynamics and statistical mechanics. Currently he leads the pan-European NOMAD project (Novel Materials Discovery)¹, which is a European Centre of Excellence that provides a central, FAIR data Repository and Archive for materials modelling. He is also pioneering in the field of big data analytics for the advancement of materials design and engineering.

Matthias Scheffler obtained his PhD in Physics from the Technical University Berlin, Germany (1978), and was then scientific staff member at the Physikalisch-Technische Bundesanstalt in Braunschweig (1978-1987). In 1979/80 he spent a year at IBM Yorktown Heights. In 1988, he became founding director of the Theory Department of the Fritz Haber Institute, where he has been since then. He is honorary professor at all three universities of Berlin and “Distinguished Visiting Professor for Materials Science and Engineering” at the University of California, Santa Barbara.

Honors and Awards (selection)

1998	Fellow of The American Physical Society
2001	Max Planck Research Award, jointly awarded by the Alexander von Humboldt Foundation and the MPG
2003	Medard W. Welch Medal and Prize, awarded by the AVS: Science and Technology of Materials, Interfaces, and Processing (formerly American Vacuum Society)
2004	Max-Born-Medal and Prize, jointly awarded by British Institute of Physics (IOP, GB) and the German Physical Society (DPG, DE)
2004-2012	<i>Visiting Professor</i> at the Dalian Institute of Chemical Physics of CAS
2007	Honorary doctorate, Faculty of Science at Lunds University, Sweden
2008	Ernst Mach Honorary Medal for Merit in the Physical Sciences, Academy of Sciences of the Czech Republic
2010	Rudolf Jaeckel Prize of the German Vacuum Society (DVG, DE)
Since 2016	<i>Visiting Professor</i> at the Institute for Catalysis, Hokkaido University, Japan
2017	Advanced Grant of the European Research Council
2017	Member of Leopoldina (German Academy of Sciences)

Synergistic Activities (selection)

- Organizer and co-organizer of numerous conferences, workshops, summer schools (about 5 per year).
- Member of the CECAM council, member of the board of directors of the node CECAM-DE-MM1P, Member of the board of trustees of psi-k, member of several scientific advisory boards.
- The computer code FHI-aims² is developed by Scheffler and his department.
- Initiator and coordinator of BiGmax³, a Max Planck research network for Big-Data Driven Materials Science.
- Initiator, founder, and chairperson of the board of the association: *FAIR Data Infrastructure for Physics, Chemistry, Materials Science, and Astronomy e.V.*⁴.

¹ <https://nomad-coe.eu/>

² <https://aimsclub.fhi-berlin.mpg.de/>

³ <https://bigmax.iwww.mpg.de/>

⁴ <http://www.fairdi.eu/>

BX-12-CLK02

Data driven discovery of new materials

Isao Tanaka

Dept. Mater. Sci. Engrg, Kyoto University, Kyoto, 606-8501, Japan, ESISM, Kyoto University, Kyoto 606-8501, Japan, MI²I, NIMS, Tsukuba 305-0047, Japan, NRL, JFCC, Nagoya 456-8587, Japan

tanaka@cms.mtl.kyoto-u.ac.jp

Keywords: materials informatics, first principles calculations, phonon anharmonicity, recommender system, chemically relevant compositions

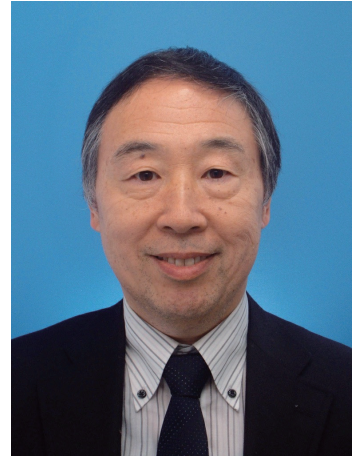
Recently, challenges for accelerated discovery of materials with the aid of data centric science have been well demonstrated. One of the approaches uses materials database that is generated by first principles density functional theory (DFT) calculations. Thanks to recent progress of computational power and technique, a large number of DFT calculations can be made with the accuracy comparable to experiments, which can be used for high throughput screening. Another approach uses machine-learning technique for making a model to estimate the target property. The whole library can then be screened. Verification process is generally required to examine the predictive power of the model. Models and the quality of the screening can be improved iteratively through Bayesian optimization process. The approach is useful when screening based upon the DFT data is not practical, i.e. when the computational cost for the descriptors is too high to cover the whole library within the practical time frame. This is the same if one needs to explore too large space to cover exhaustively. As an example of the use of a machine learning model to screen a library, I will talk about the story on the discovery of new low lattice thermal conductivity (LTC) crystals [1]. We have established our own LTC dataset computed by the first principles anharmonic force constant method [2]. Using approximately 100 theoretical LTC data, we made a machine learning model for LTC. Then all compounds registered in the inorganic crystal structure database (ICSD) library were ranked with respect to the predicted LTC. Finally, the candidates of the low LTC compounds were validated by first principles LTC calculations. A variety of compounds showing ultra-low LTC of approximately 0.1 Wm/K at 300 K were thereby discovered.

In the second part of my talk, I will explain matrix- and tensor-based recommender system using information of compounds registered in ICSD. It was found to be very powerful for discovery of currently unknown chemically relevant compositions (CRCs) of inorganic compounds from vast candidates [3]. The discovery rate was evaluated by the presence of highly-rated chemical compositions in the other databases of experimentally known compounds, i.e., ICDD-PDF and Springer Materials, excluding CRCs registered in ICSD. For ternary and quaternary compositions, the rate was approximately 60% and 50% for the top 100 compositions, respectively. The high discovery rate with neither DFT database nor other prior physical/chemical knowledge should be noteworthy.

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Isao TANAKA is Professor in the Department of Materials Science and Engineering, Kyoto University, Japan. Trained as a metal physicist, he received his B.E. and M.E. from Kyoto University and his Ph.D. from Osaka University. In 1987, he joined ISIR, Osaka University, as an assistant professor where he studied processing and characterization of high purity silicon nitride. He got an Alexander von Humboldt Fellowship in 1992 and stayed a year in Manfred Rühle's research group of Max Planck Institute for Metals Research in Stuttgart, Germany, where he studied intergranular glassy films of silicon nitride ceramics. He returned to Kyoto University in 1993 and started to use quantum mechanical calculations and combined them with experimental techniques such as ELNES and XANES to study fundamental issues in a wide range of ceramic materials. He also studied electronic processes of defects, impurities, grain boundaries, surfaces, and their roles in macroscopic properties. In 2000s he made pioneering studies on theoretical calculation of thermo-physical properties of ceramic materials through first principles phonon calculations. Recently he is actively working on data-centric or informatics approach for discovery of new materials. Materials of his current interests are quite diverse including solid-state ionics, battery materials, oxide/nitride semiconductors, engineering ceramics, etc. He is author or coauthor of 411 papers and holds *h*-index of 56. Recently he edited a book titled *Nanoinformatics* (Springer).



BX-12-CLK03

Geometric frustration and the intrinsic approach in material science

*Efi Efrati¹

¹Weizmann Institute of Science, Rehovot, 76100, Israel,

*efi.efrati@Weizmann.ac.il

Keywords: elasticity, geometric frustration, residual stress, incompatibility.

Unlike Lego bricks that perfectly assemble next to one another, in many molecular assemblies and modern applications of responsive materials some misfit is almost always present. The constituents of such structures must distort in order to fit next to one another resulting in geometrically frustrated structures that possess no stress-free rest state. The elastic behavior of such structures is thus best described through local intrinsic geometric quantities such as their metric.

In this talk, I will survey how the intrinsic approach is implemented to describe frustrated thin sheets known as non-Euclidean plates, twisted molecular crystals, and two-dimensional liquid crystals. The intrinsic approach predicts the striking variety of morphologies of ground states and exotic response properties such structures exhibit, and moreover allows to better engineer self-shaping responsive structures.

Efi Efrati
Curriculum Vitae

Contacts
efi.efrati@weizmann.ac.il
Department of physics of complex systems
Weizmann Institute of Science
PO Box 26, Rehovot 76100
Israel



Academic employment and education

2014-present	Assistant professor, Weizmann institute of Science.
2010-2014	Simons Postdoctoral fellow, James Franck Institute, The university of Chicago.
2005-2010	Ph.D, Racah Institute of Physics, The Hebrew University Jerusalem. Summa cum laude.
2003-2005	M.Sc, Racah Institute of Physics, The Hebrew University Jerusalem.
2001-2003	B.Sc. Physics and Mathematics, The Hebrew University of Jerusalem. Magna cum laude.

Fellowships and awards

2016-present	Incumbent of the Ernst and Kaethe Ascher Career Development Chair.
2014-2017	Alon Fellowships for Outstanding Young Researchers.
2013	Compton lectureship, University of Chicago.
2011	The Hebrew University Max Schlomiuk award for outstanding PhD thesis.
2010-2013	Simons post-doctoral fellowship.
2010	Rothschild post-doctoral fellowship (declined).
2004	Giulio Racah prize for theoretical physics (M.Sc)

CX-13-CLK01

Evolution of LPSO Structure to Mille-Feuille Structure in Ultrahigh-Strength Magnesium Alloys

*Yoshihito Kawamura¹

¹Magnesium Research Center (MRC), Kumamoto University, Kumamoto, 860-8555, Japan

*rivervil@gpo.kumamoto-u.ac.jp

Keywords: Magnesium, LPSO structure, Kink Strengthening, Mille-feuille structure, Structural materials

Mg alloys are attractive for use in aircraft components primarily because of their low density and high specific strength. But current commercial Mg alloys, e.g., AZ31, have low yield strength and unacceptably low ignition temperature. Moreover, several years ago America's FAA (Federal Aviation Administration) has lifted the ban on the use of some Mg alloy forms in the payload area and has set up a standardized testing method of flammability for Mg alloys¹⁾. In addition, biodegradable tailored Mg alloys are some of the most promising scaffolds for cardiovascular stents.

Ultrahigh-strength Mg-M-RE (M is Co, Ni, Cu or Zn, and RE is Y, Gd, Tb, Dy, Ho, Er or Tm) alloys with high heat-resistance and great flame-resistance have been developed at Kumamoto University in Japan and are now a world leading focus of Mg R&D²⁾³⁾. These Mg-M-RE alloys, which are composed of alpha Mg phase and LPSO phase having a long-period stacking ordered (LPSO) structure, are called LPSO-type Mg alloys because their main strengthening phase is the LPSO phase⁴⁾. The LPSO phase is strengthened by kinking, which is a new concept for strengthening mechanism of metals. The LPSO-type Mg-M-RE alloys, which were produced by hot extrusion of cast ingot, exhibited very high symmetrical yield strength in both tension and compression, high heat resistance, and great flame resistance. A small amount addition of Al and La improved the corrosion resistance, resulting in the same as the commercial AZ31 alloy. Moreover, the ignition temperature was improved by a small amount addition of Be, Yb or Ca, resulting in high ignition temperature above 1200 K. A rapidly solidified powder metallurgy (RS P/M) method, where rapidly solidified powder or ribbons are consolidated by hot extrusion, improved the mechanical and corrosion properties as compared with ordinary ingot metallurgy (I/M) method, where cast ingot is hot extruded. The development of more sustainable and more affordable manufacturing technology for these next-generation Mg alloys has been conducted via an integrated and comprehensive collaboration between academia and industry. Moreover, the applications and commercialization of these advanced Mg alloys have been under serious investigation and study for automobile, aircraft, and biomedical industries. In the LPSO structure, L1₂-type M₆RE₈ cluster layer with 4 atomic planes and Mg layer with 1~4 atomic planes are orderly stacked. The former L1₂-cluster layer is hard and the later Mg layer is soft; thus resulting in an ordered stacking structure of hard and soft layers within the LPSO structure. We have, therefore, named these kinds of stacking structure of hard and soft layers "mille-feuille structure" after mille-feuille pastry having a stacking structure of pie and cream layers. Recently, we have discovered a new class of magnesium alloys with this kind of mille-feuille structure, in which stacking faults, composing of a single layer of L1₂-cluster, are sparsely distributed in alpha-Mg matrix. The new magnesium alloys were strengthened by kinking as well as LPSO phase, and they exhibited a greater mechanical strength than the LPSO-type Mg alloys. In my presentation, I will report the features of the performances and microstructure of the LPSO-type Mg alloys and introduce the new discovery of the mille-feuille structure.

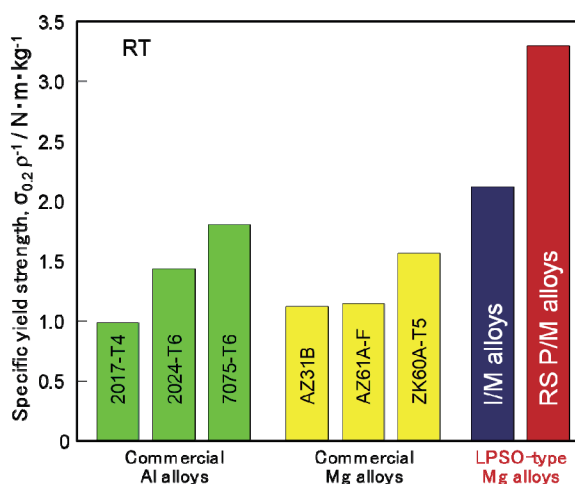


Fig. 1. Specific tensile yield strength of LPSO-type Mg alloys produced by I/M and RS P/M methods.

References:

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Yoshihito Kawamura (ph.D)

Date of birth: August 20,1960

Nationality: Japan

Director, Magnesium Research Center, Kumamoto University
Kuro-kami 2-39-1, Chuo-ku, Kumamoto 860-8555, Japan



Biosketch:

Professional Career

Dec. 2011 -To date	Director, Magnesium Research Center, Kumamoto University
Apr. 2004 – To date	Professor, Graduate School of Science and Technology, Kumamoto University
Oct. 2000 – Mar. 2004	Associate Professor, Graduate School of Science and Technology, Kumamoto University
Sep. 1999 - Sept. 2000	Associate Professor, Institute for Materials Research, Tohoku University
Apr. 1993 – Aug. 1999	Associate Researcher, Institute for Materials Research, Tohoku University
Apr. 1985 – Nov. 1989	Researcher, R&D Department, Nippondenso Co., Ltd

Academic Career

Mar. 1993	Doctor of Engineering, Tohoku University (ph. D)
Mar. 1985	Master of Engineering, Nagoya University
Mar. 1983	Bachelor of Engineering, Nagoya University

Major Awards

- The Medal of Honor with Purple Ribbon, Cabinet office of Japan (2017)
- The JIM Distinguished Contribution Award, Japan Institute of Metals and Materials (2015)
- The "HONDA" Frontier Award, The Honda Memorial Foundation (2013)
- The "NISTEP" Award (The Researchers with Nice Step), MEXT (2012)
- The "SOKEIZAI" Industry Technology Award, Sokeizai Center (2009)
- The "MONOZUKURI RENKEI" Award, The Nikkan Kogyo Shinbun Ltd. (2008)
- The JIM Meritorious Award, Japan Institute of Metals and Materials (2000)

Other Academic and Professional Activities

- Science Council of Japan (Member, 2014-to date)
- The Japan Institute of Metals and Materials (Director, 2012-2014)
- The Japan Institute of Light Metals (Director, 2015-2018)
- The Japan Magnesium Association (Director, 2017-to date)
- The Kyushu Magnesium Network (President, 2004-to date)
- MEXT "KAKENHI" Program of Grant-in-Aid for Scientific Research on Innovative Areas, "Materials Science of Synchronized LPSO Structure" (Project leader, 2011-2016)
- JST "CREATE" Program (Project leader, 2008-2011)

Publications:

- Published papers: 306 (from SCOPUS)
- Citation: 12,166 (from SCOPUS)
- h-index: 59 (from SCOPUS)

CX-13-CLK02

Additive Manufacturing of Ceramic Components with Unique Structures

*Tatsuki Ohji

National Institute of Advanced Industrial Science and Technology (AIST), Nagoya 463-8560, Japan

* t-ohji@aist.go.jp

Keywords: Additive manufacturing, Ceramics, Components, Powder

Aiming for innovative ceramic manufacturing technologies which enable creative and novel products, a national R&D project “High-Value Added Ceramic Products Manufacturing Technologies (HCMT)” has been initiated since 2014 with 5-year scheme (2014-19) as a part of SIP “Innovative design/manufacturing technologies” program in Japan. The project deals with two key technologies: additive manufacturing (AM) for realizing complex-shaped ceramic products and reducing their lead-times, and hybrid coating on 3D bodies for enhancing their functionality and durability. Following an overview of this project and a brief description on the general status of AM technologies, this talk focuses on the R&D strategies and the final achievements on AM of ceramics in this project. Among a variety of AM approaches, we have employed two AM technologies for making ceramic green bodies; powder layer manufacturing (powder bed fusion or indirect selective laser sintering) and slurry layer manufacturing (vat photo-polymerization or stereolithography), because of their dimensional accuracy, shape-flexibility, density-adjustability, *etc.* The former is a dry forming process, and is suitable for large/porous components, while the latter is a wet one, being good for small/dense parts. In addition, intensive research efforts have been devoted to ceramic laser sintering (direct selective laser sintering) which enables concurrent forming and sintering (saving post-sintering-process). This paper describes several 3D prototype models produced for various application targets using the developed AM technologies, which have unique and complicated structures never attainable with conventional methods. The current issues and future perspective for AM of ceramics will be addressed and discussed as well.

This work was conducted as a part of “High-value added ceramic products manufacturing technologies project” supported by CSTI, SIP, “Innovative design/manufacturing technologies (managed by NEDO)”.



Tatsuki Ohji is a Fellow of National Institute of Advanced Industrial Science and Technology (AIST), Japan. BS and MS in mechanical engineering from Nagoya Institute of Technology and Ph. D. in inorganic materials engineering from Tokyo Institute of Technology, he has authored or coauthored more than 350 peer-reviewed papers and 20 book chapters, edited more than 40 books and conference volumes, and chaired or co-chaired more than 40 international conferences and symposia. His research interests include mechanical property characterization of ceramics, ceramic composites and porous materials, microstructural design of ceramic materials for better performance, structural control of meso/ macro porous ceramics, and green manufacturing of ceramic components. Fellow of the American Association for the Advancement of Science (AAAS), The American Ceramic Society, ASM International, the Ceramic Society of Japan, and the European Ceramic Society and Academician of the World Academy of Ceramics, he has received numerous awards including John Jeppson Award, Samuel Geijsbeek PACRIM International Award, and ECD Bridge Building Award all from The American Ceramic Society, Academic Achievement Award from the Ceramic Society of Japan, IIM Lectureship Award from ASM International, Honour Medal of Aurel Stodola from the Slovak Academy of Science, Lee Hsun Lecture Award from Chinese Academy of Sciences, and Distinguished Research Achievement Award from the Japan Society of Powder and Powder Metallurgy. He currently serves as President of the American Ceramic Society and an Editor of “Journal of the American Ceramic Society” and “Ceramic International” in addition to an editorial board member of many international journals.

CX-13-CLK03

Detecting bond scission in fracture of soft materials

Juliette Slooman^a, Josh Yeh^a Robert Goestl^c and Costantino Creton^{a,b}

^aLaboratoire SIMM, ESPCI Paris, CNRS, PSL University, Paris, France. ^bGlobal Station for Soft Matter, University of Hokkaido, Japan. ^cDWI - Leibniz-Institut für Interaktive Materialien, RWTH Aachen, Germany

Fracture of soft materials is a complex process coupling non linear mechanics and statistical physics¹⁻². Because of the large deformations involved before a crack propagates, molecular damage typically occurs in the bulk of the material and not only in the fracture plane³. This is particularly true for tough soft materials where bulk energy dissipation mechanisms such as sacrificial bonds are introduced by design. Until recently the detection of damage ahead of a crack was limited to the detection of crystallization or cavitation, detectable by wide or small angle X-ray scattering or optical visualisation, but molecular bond scission was not directly detectable. However organic chemists have now developed several molecules that respond to applied forces or bond scission by changing their light absorption or emission properties⁴⁻⁶ providing novel opportunities for materials scientists to gain insight in molecular processes occurring during mechanical loading.

We have incorporated mechanosensitive fluorophore molecules⁴ as crosslinkers in model transparent elastomers and studied how these bonds break during macroscopic fracture. Pi-extended anthracene based molecules can be used to obtain high resolution spatial information and the extent of damage can be quantified with suitable calibration samples. We will focus in this talk on the strain rate and temperature dependence of the molecular bond scission in simple networks and demonstrate how the extent of molecular irreversible damage during fracture is highly dependent on the viscoelastic effects.

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CV Costantino Creton

Dean of Research of [ESPCI Paris](#)
 CNRS Directeur de Recherche at
[Laboratory of Soft Matter Science and Engineering](#),
 Distinguished Professor at University of Hokkaido
 Scientific Chair of Dutch Polymer Institute
E-mail: Costantino.creton@espci.fr
Web : <http://ccreton.simm.espci.fr/>



Research interests:

mechanical properties of elastomers, deformation, adhesion and fracture of soft polymer networks.
 mechanochemistry; mechanical properties of hydrogels.

Biographic description:

Costantino Creton graduated in Materials Science from the [Ecole Polytechnique Fédérale de Lausanne \(Switzerland\)](#) in 1985. He then moved on to the [Materials Science and Engineering Department of Cornell University](#) (USA) where he obtained his Ph.D in 1991. After a post-doc at the [IBM Almaden Research Center](#) (USA), he joined the [ESPCI Paris](#) first as a post-doctoral associate in 1993 and, since 1994 as a C.N.R.S. permanent researcher. He was promoted CNRS research director (equivalent to Professor) in 2001 in the [Laboratory of Soft Matter Science and Engineering](#). Since 2019 he is the Dean of Research of the ESPCI Paris

He also holds since 2011 the position of scientific director of the [ESPCI Paris](#), scientific chairman of the [Performance Polymers technology area of the Dutch Polymer Institute](#) and has been appointed in 2016, Distinguished Professor at the [Global Station for Soft Matter](#) of [Hokkaido University](#).

He has published more than 180 articles in peer-reviewed journals, nine book chapters and has given more than 110 invited and plenary lectures at international conferences. He has received several prizes and awards including the [Wake Medal](#) from the UK Society of Adhesion and Adhesives in 2011 and the Adhesion Society's [prize for Excellence in Adhesion Science](#) in 2013. He was also elected in 2013 [fellow of the American Physical Society](#) and received an ERC Advanced Grant in 2016 to work on fracture of soft materials.

DX-12-CLK01

Atomic-level control of high temperature superconductor materials for unveiling their pairing mechanism

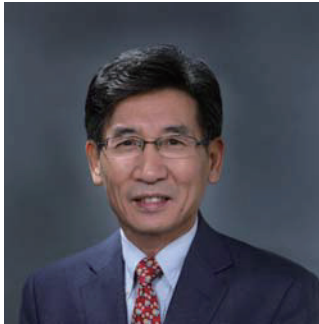
Qi-Kun XUE

Tsinghua University and Beijing Academy of Quantum Information Sciences, Beijing, China

Email: qkxue@mail.tsinghua.edu.cn

Keywords: superconductors, molecular beam epitaxy, scanning tunneling microscopy

We investigate the pairing mechanism of high T_c superconductivity in cuprates and iron-pnictides by using state-of-the-art molecular beam epitaxy (MBE)-scanning tunneling microscopy (STM), angle-resolved photoemission spectroscopy and Josephson tunneling experiment. By MBE growth, we are able to prepare superconducting CuO_2 planes in BSCCO and LSCO and FeSe planes in Fe-based pnictides, which provides an unprecedented opportunity to investigate the pairing mechanism in well-controlled manner. We show that the pairing symmetry in both systems is rather conventional. We propose a model for understanding the complicated phase diagram and mechanism of unconventional high temperature superconductivity in the two systems.



Prof. Qi-Kun Xue 薛其坤

Department of Physics, Tsinghua University, B409, New Science Building

Email: qkxue@mail.tsinghua.edu.cn

Phone: +86 10 62795618

Education

1994 Institute of Physics, Chinese Academy of Sciences (CAS), Ph.D in physics.

Employment

2017 – present Director, Beijing Academy of Quantum Information Sciences.

2013 – present Vice President for Research, Tsinghua University.

2013 – 2014 Dean, Office of Scientific Research and Development, Tsinghua University.

2011 – present Director, State Key Laboratory of Low-Dimensional Quantum Physics.

2010 – 2013 Chair, Department of Physics, Tsinghua University.

2010 – 2013 Dean, School of Sciences, Tsinghua University.

2005 – present Distinguished Professor, Department of Physics, Tsinghua University. 1999 –

2005 Director, State Key Laboratory for Surface Physics, Institute of Physics, CAS.

1999 – 2007 Professor, Head of Group SF04, State Key Laboratory for Surface Physics, Institute of Physics, CAS.

1994 – 1999 Research Associate, Institute for Materials Research, Tohoku University.

Honors

2016 Future Science Prize-Physical Science Prize

2014 Asian Union of Magnetism Societies Award.

2014 HLHL Achievement Award in Science and Technology.

2014 Qiu Shi Outstanding Scientist Award.

2013 Distinguished Talent of 10000 Talents (Wanren) Program.

2012 Tan Kah Kee Science Award in Mathematic and Physical Sciences.

2011 National Natural Science Award (Second-class) of China.

2011 Qiu Shi Outstanding Scientific Research Team Award.

2010 TWAS Physics prize.

2006 HLHL Advancement Award in Science and Technology.

2005 Member of the Chinese Academy of Sciences.

2005 Cheung Kong Distinguished Professor, Ministry of Education.

2005 Outstanding Achievement Award in Science and Technology, CAS.

2004 National Natural Science Award (Second-class) of China.

2004 Young Scientist Prize, the Chinese Association of Science and Technology.

1998 100 Talents Program, the Chinese Academy of Sciences.

1997 Young Scientist Fund, National Natural Science Foundation of China.

1994 President Prize for Excellent PhD Students, CAS.

DX-12-CLK02

Development of Corundum-Structured Gallium Oxide Power Devices by MIST EPITAXY®

*T. Shinohe

FLOSFIA Inc., Kyoto, 615-8245, Japan

*shinohe@flosfia.com

Keywords: Power device, Ga₂O₃, MIST EPITAXY®, corundum family, SBD, MOSFET

For several decades the power electronics industry has relied on Si semiconductor devices. However, the physical limitations of Si have triggered the development of wide bandgap semiconductors, including SiC (E_g = 3.3 eV) and GaN (E_g = 3.4 eV). On the other hand, it is reported that corundum-structured Ga₂O₃ (α-Ga₂O₃) (E_g = 5.3 eV), which is one of the metastable phases in Ga₂O₃ polymorphs, thin films can be obtained by mist chemical vapor deposition (mist-CVD) ¹⁾. Using inexpensive sapphire substrates and mist CVD growth technique, there is a possibility to fabricate Ga₂O₃ devices at low cost.

Gallium oxide takes five different phases (α, β, γ, δ, and ε). The orthorhombic β-gallia structure (β-phase) is the most stable crystal structure ²⁾, and corundum-structure (α-phase) has the widest bandgap among them. As shown in Table 1 and Figure 1, the breakdown electric field (E_c) of α-Ga₂O₃ is about 30 times that of Si and 4 times that of SiC, and that offers the following advantages of α-Ga₂O₃ power devices over counterparts: (1) the thickness of the drift layer of α-Ga₂O₃ can be reduced to 1/30 of that of Si and 1/4 of that of SiC, and also higher doping is possible to the drift layer of α-Ga₂O₃, those combined enable reduction of the drift layer resistance to 1/340 that of Si and 1/6726 that of SiC in unipolar devices; and (2) the use of the same drift layer thickness enables a blocking voltage of 30 times that of Si and 4 times that of SiC. The characteristics (1) would enable further reduction of the on-resistance of unipolar devices. The characteristics (2) would enable the fabrication of devices operating at ultra-high blocking voltages (> 10 kV) and it would be possible to reduce the number of series connected devices required for construction of high power converter systems. Further, the wide bandgap of α-Ga₂O₃ (E_g = 5.3 eV) enables high temperature operation.

In this paper, the development status of Corundum-Structured Gallium Oxide Power Devices, such as SBD ³⁾ and MOSFET ⁴⁾ will be presented.

Acknowledgements:

Part of this work was supported by “Strategic Innovation Program for Energy Conservation Technologies” of the New Energy and Industrial Technology Development Organization (NEDO).

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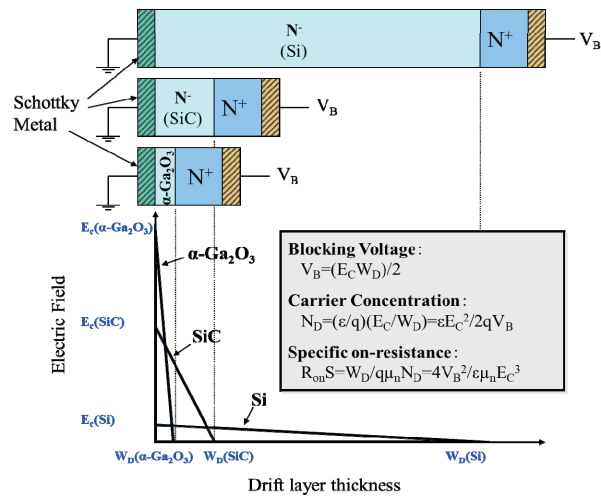


Fig. 1. The reason why low on-resistance can be attained.

Table 1. Comparison of physical properties with competing materials.

Name of material	Si	4H-SiC	GaN	β-Ga ₂ O ₃	α-Ga ₂ O ₃ (Corundum structure)	
Bandgap E _g (eV)	1.1	3.3	3.4	4.5	5.3	
Mobility μ (cm ² /Vs)	1,400	1,000	1,200	300	300 (estimate)	
Dielectric breakdown field E _c (MV/cm)	0.3	2.5	3.3	7	10 (estimate)	
Relative dielectric constant	11.6	9.7	9.0	10	10 (estimate)	
Baliga's figure of merit Sj = 1	Low frequency (μE _c ²)	1	340	870	2,307	6,726 (estimate)
	High frequency (μE _c ³)	1	50	104	117	238 (estimate)

**Biography:**

CTO & Director of FLOSFIA Inc.

Fellow, The Institute of Electrical Engineers of Japan (IEEJ)

He had been contributing in many research & development activities on Silicon (Si) and Silicon Carbide (SiC) power devices (SBD, PiN, JFET, MOSFET, IGBT) and their applications (Inverter & Converter for trains) in Toshiba Research and Development Center over 35 years. In addition, he has participated in many national projects on power devices. He joined FLOSFIA Inc. in 2017, and is directing research and development of corundum-structured Ga₂O₃ power devices as CTO & Director.

DX-12-CLK03

Emergent electromagnetism in quantum materials

*N. Nagaosa^{1,2}

¹ RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama 351-0198, Japan, ² The University of Tokyo, Tokyo 113-8656, Japan

* nagaosa@riken.jp

Keywords: spin textures, spin-orbit interaction, Berry phase

Most of the physical properties of materials are formulated in terms of the electromagnetic responses. Electrical transport, magnetism, optical properties, dielectric response, superconductivity are all related to the responses of the materials to the electromagnetic field. Therefore, electromagnetism offers a fundamental of materials science. In this talk, I will discuss a new electromagnetism formulated for electronic systems in solids due to their quantum nature. Namely, the manifolds in Hilbert space are characterized by the connection and curvature, which correspond to vector potential and field strength of electromagnetic field, respectively. This geometric picture provides a predicting power for various properties of materials leading to the design of their functions.

Especially in magnets, it often happens that the spin structure is non-collinear as shown in Fig.1. With the tilting of the spins, the quantum mechanical amplitude for the hopping of a conduction electron between the two sites gains a phase factor analogous to the vector potential. This vector potential leads to the emergent electromagnetic field in real space. For example, the three spins subtending a solid angle produce an emergent magnetic field leading to the Hall effect.

Various effects viewed from this emergent electromagnetism will be discussed including the nonreciprocal transport and rectification effect, nonreciprocal photovoltaic effects with possible application to solar cell, various Hall responses, multiferroics for insulator spintronics, and nano-scale inductor made from spiral magnets.

References (Example: non-mandatory, 10 point):

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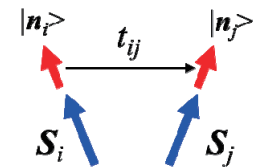


Fig. 1. Spin texture with tilting angle leads to the vector potential \mathbf{a} for the transfer integral of conduction electrons.

Curriculum Vitae Naoto Nagaosa

Deputy Director

RIKEN Center for Emergent Matter Science

RIKEN-ASI, Wako, Saitama 351-0198, Japan

Tel: +81-48-467-9603 E-mail: nagaosa@riken.jp

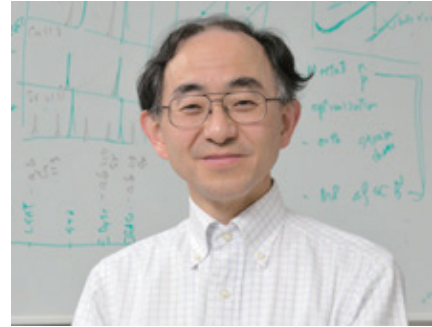
Professor

Department of Applied Physics,

The University of Tokyo,

7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

Tel: +81-3-5841-6811 E-mail: nagaosa@ap.t.u-tokyo.ac.jp



– Date of birth: February 21, 1958

– Education:

1980 B. S. Dept. of Applied Physics, University of Tokyo

1980–1983 Graduate School of Engineering, University of Tokyo

– Degrees:

1986 University of Tokyo, Ph.D (Physics)

– Appointments:

1983–1986 Research associate, Theory division, Institute for Solid State Physics, University of Tokyo

1986–1989 Research associate, Department of Applied Physics, University of Tokyo

1989–1993 Lecturer, Department of Applied Physics, University of Tokyo

1993–1998 Associate professor, Department of Applied Physics, University of Tokyo

1998– Professor, Department of Applied Physics, University of Tokyo

2001–2007 Team Leader, Theory Team, Correlated Electron Research Center, Advanced Industrial Science and Technology

2007–2013 Team Leader, Theoretical Design Team, RIKEN

2010–2013 Team Leader, Strong-Correlation Theory Research Team, RIKEN

2013– Deputy Director, RIKEN Center for Emergent Matter Science (CEMS),
Division Director, Strong Correlation Physics Division, RIKEN CEMS
Group Director, Strong Correlation Theory Research Group,

EX-11-CLK01

Antiferromagnets for neuromorphics and opto-electronics

*Tomas Jungwirth^{1,2}

¹ Institute of Physics, Academy of Sciences of the Czech Republic, Czech Republic, ² School of Physics and Astronomy, University of Nottingham, United Kingdom

* jungw@fzu.cz

Keywords: antiferromagnets, spintronics, memories, neuromorphics, opto-electronics

Louis Néel pointed out in his Nobel lecture that while interesting from theoretical viewpoint, antiferromagnets did not seem to have any applications. Indeed, the alternating directions of magnetic moments on individual atoms and the resulting zero net magnetization have made antiferromagnets hard to control by tools common in ferromagnets. This has hindered both the research and utility of these abundant magnetic materials. Recent studies have shown, however, that current-induced spin-orbit torque and anisotropic magnetoresistance can be used to efficiently manipulate and detect the Néel vector (1). Switching signals in these first realizations of antiferromagnetic memories were in the fraction of a per cent scale – far from the requirements for practical applications. We will present a concept showing alternative means for electrical or optical switching, spanning a broad range from microseconds to femtoseconds, in memory devices comprising a simple film of an antiferromagnet and showing readout signals in the ~10-100% range. We fabricate analogue memory micro-devices with remarkably reproducible, reversible multi-level switching signals that are insensitive to magnetic fields. Our concept should be generally applicable to the broad family of stray-field-free antiferromagnets and opens research and development directions ranging from microelectronic memory-logic components for spiking neural networks to opto-electronic memory-sensor devices with high temporal and spatial resolution.

References:

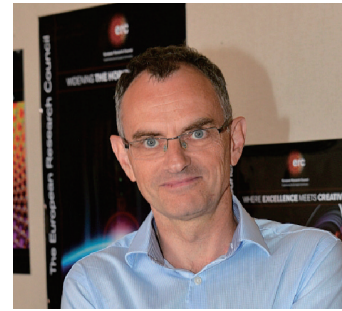
1) Focus on Antiferromagnetic Spintronics, Nature Physics 14 (2018).

Curriculum Vitae

Tomáš Jungwirth

Born: October 23, 1967, Praha, Czech Republic

Home page: <http://www.fzu.cz/~jungw>



Education and professional career:

- | | |
|--------------|---|
| 2007-present | Head of the Department of Spintronics and Nanoelectronics, Institute of Physics, Academy of Sciences of the Czech Republic (ASCR) |
| 2004-present | Professor, University of Nottingham, UK |
| 2001-2007 | Senior Research Scientist, Institute of Physics ASCR |
| 2000-2002 | Research Fellow, University of Texas, USA |
| 1997-1999 | Postdoctoral Fellow, Indiana University, USA |
| 1997 | PhD. degree in condensed matter physics, Charles University, Czech Republic |
| 1991 | M.S. degree in physics, Charles University, Czech Republic |

Professional experience:

condensed matter physics; materials science; collective phenomena; electronic properties of semiconductor heterostructures, low-dimensional systems, and nanostructures; quantum Hall effects; carrier-mediated ferromagnetism in diluted magnetic semiconductors; magnetic, magneto-transport and magneto-optical properties of ferromagnetic semiconductors; spin-orbit coupling phenomena; anisotropic magnetoresistance in magnetic bulk and nano-devices; anomalous and spin Hall effects; non-magnetic, ferromagnetic, and antiferromagnetic metal and semiconductor spintronics

Accomplishments, awards, memberships:

- 225 publications, including 4 in Reviews of Modern Physics, 29 in Physical Review Letters, 30 in Nature/Science family journals; h-index 54 (WoS); ~ 12, 000 citations (~ 1, 500 in 2017); ~ 150 invited talks at international conferences and colloquia since year 2000
- Member of the Scientific Council of the European Research Council, 2015-
- Member of the Academy of Europe (Academia Europaea), 2014-
- European Research Council Advanced Grant, 2011-2016
- Member of the European Research Council Evaluation Panel, 2009-2015
- Praemium Academiae, 2008-2014
- Academy of Sciences of the Czech Republic Prize, 2005
- Otto Wichterle Prize of the Academy of Sciences of the Czech Republic, 2002
- NATO-NSF Advanced Fellowship, 2000
- Bolzano Foundation Prize of the European Physical Society, 1996
- Josef Hl'avka Prize, 1996
- Milan Odehnal Prize of the Union of Czech Mathematicians and Physicists, 1996

EX-11-CLK02

Quantum Criticality in Organometallics Studied by Neutrons & Muons

*Martin Månsson¹

¹ Department of Applied Physics, KTH Royal Institute of Technology, Stockholm, Sweden

*condmat@kth.se

Keywords: quantum magnetism, neutron scattering, muon spin spectroscopy

Quantum phase transitions have been in the center of attention for scientists world-wide to understand the universality of quantum critical behavior in many-body systems. Gapped Heisenberg spin- $\frac{1}{2}$ systems have the potential to exhibit quantum critical phenomena in their excitation spectra as a function of *e.g.* magnetic field and pressure. In such compounds, tuning of the spin gap exercises a control of the ground state and enables the study of novel fundamental many-body phenomena. In this keynote I will give a brief overview on how we are able to build tailored spin compounds using organometallic frameworks and how to experimentally study their intrinsic properties using complementary neutron [1-3] and muon [4] techniques. Further, I will show how it is possible to induce quantum criticality in the quantum spin-liquid compound $[\text{C}_4\text{H}_{12}\text{N}_2][\text{Cu}_2\text{Cl}_6]$ using both magnetic field and hydrostatic pressure. Finally, I will also show future extensions for how to use an organic materials data base (OMDB) and advanced machine learning to model, search and identify future interesting compounds for targeted synthesis and characterizations [5,6].

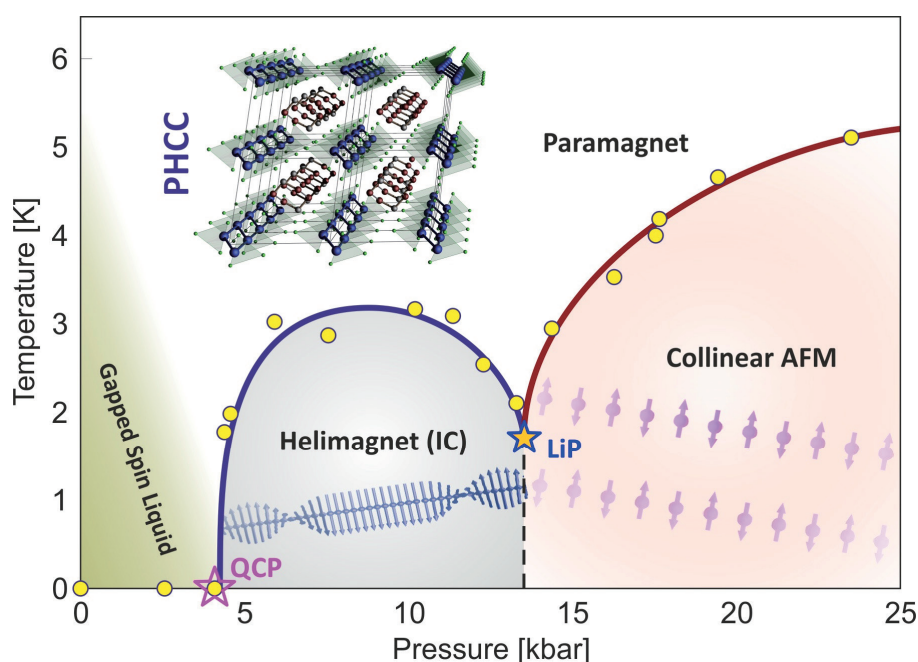


Figure 1: Pressure-Temperature phase diagram for the quantum spin-liquid compound $[\text{C}_4\text{H}_{12}\text{N}_2][\text{Cu}_2\text{Cl}_6]$, also known as Piperazinium hexachloro - dicuprate (PHCC)

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- [4] M. Thede, M. Månsson, *et al.*, *Physical Review Letters* **112**, 087204 (2014)
- [5] <https://omdb.mathub.io/> [2019]
- [6] J. Hellsvik, M. Månsson, A.V. Balatsky, *et al.*, arXiv:1907.01817

Your Portrait:



Your C.V.

Martin Månsson is an experimental physicist with a PhD in materials physics from KTH Royal Institute of Technology in Stockholm with a thesis focusing on angle-resolved photoelectron spectroscopy (ARPES) investigations of correlated electron systems, *e.g.* high-temperature superconductors (HTSC). Subsequently he spent seven years in Switzerland as a postdoc and scientist at the Paul Scherrer Institute (PSI), ETH Zurich and EPF Lausanne. Here he focused on studying novel energy materials (in collaboration with Toyota Central R&D Labs.) as well as quantum magnetism using neutron scattering and muon spin rotation/relaxation (μ^+ SR) techniques. Since 2015 he has returned to Stockholm and KTH where he is currently holding a tenured Assoc. Professor position in Applied Physics as well as Neutron Scattering. In addition to running a comprehensive research program on both sustainable energy materials as well as strongly correlated electron physics he is also highly involved in the strategic developments and educational efforts connected to the construction of the European Spallation Source (ESS) in Sweden. Among other things, he is *e.g.* the Director of Studies for the Swedish national graduate school in neutron scattering (SwedNess).

EX-11-CLI03

Probing antiferromagnets with currents

O. Gladii¹, R. L. Seeger¹, L. Frangou¹, G. Forestier¹, A. Hallal¹, P. Noël¹, S. Auffret¹, M. Rubio-Roy¹, I. Joumard¹, L. Vila¹, M. Chshiev¹, C. Gomez², S. Gambarelli³, M. Houzet⁴, *V. Baltz¹

¹ SPINTEC - Univ. Grenoble Alpes / CNRS / CEA / GINP, Grenoble, 38000, France ² SYMMES - Univ. Grenoble Alpes / CEA, ³ CIME Nanotech – GINP, ⁴ Pheliqs - Univ. Grenoble Alpes / CEA

* vincent.baltz@cea.fr

Keywords: antiferromagnets, spin fluctuations, spin-charge conversion

The paradigm shift consisting of using the spin-dependent transport properties of antiferromagnets in electronics led to many exciting challenges.^{1,2)}

In this talk, we will first discuss the nature of a spin current flowing through fluctuating antiferromagnets and distinguish between electronic and magnonic spin transport. The method used to inject the spin currents involved ferromagnetic resonance and spin pumping in ferromagnetic-spin-injector/(non-magnetic-spin-conductor)/antiferromagnetic-spin-sink multilayers. Three typical cases will be presented, magnonic spin flow in the insulating antiferromagnets NiO and NiFeOx, electronic spin flow in the metallic antiferromagnet IrMn, and electronic and magnonic parallel spin flows in IrMn when the latter is directly exchange coupled to the ferromagnetic-spin-injector. In this latter case, how it is possible to unravel the spin injection efficiency of the two types of spin flows will be demonstrated. We will also demonstrate how linear spin fluctuations enhance spin injection in spin-sinks (Fig. 1) and show why this is pertinent for studies of critical phenomenon like magnetic phase transitions in ultra-thin films. To show the far-reaching practical relevance of the method, extension to various phase transitions will be presented.³⁻⁶⁾ In search for spin fluctuations in several antiferromagnetic spin-sinks, we will also discuss how we found experimental evidence of self-induced spin-charge conversion in the spin-injector, corroborating the results of first-principle calculations.^{7,8)} Beyond spin currents, we will finally present a stimulating example of how antiferromagnets and superconductors may envision a common future by showing how to infer essential information about domain walls using Cooper pairs through antiferromagnets.^{9,10)}

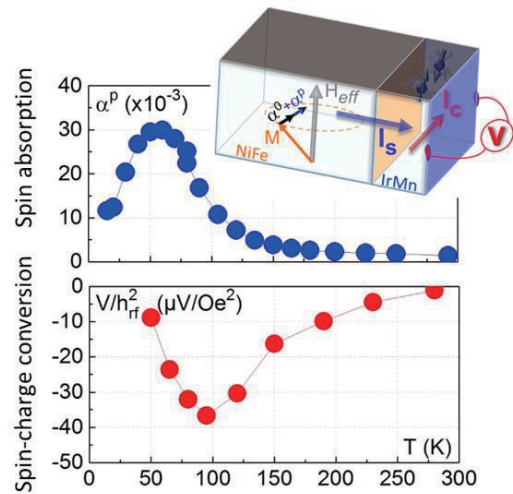


Fig. 1. Increased spin absorption due to the spin fluctuations of the absorber near its magnetic phase transition (here, the IrMn antiferromagnet). The expected increase of the spin-charge conversion in the absorber is masked by self-induced conversion in the injector (here, the NiFe ferromagnet).

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BALTZ Vincent

Vincent Baltz (born 1979) received the Ph.D. degree in physics in 2005 and the H.D.R. 'Habilitation à diriger des recherches' degree in physics in 2014 from the University of Grenoble, France. He has been conducting research in magnetism and spintronics with SPINTEC since 2007 as a C.N.R.S. research scientist. Before that, he was a post-doctoral fellow at the University of Leeds in the condensed matter group in the frame of a Marie-Curie European research training network.



His research interests include magnetic heterostructures with current focus on antiferromagnetic spintronics. His fields of expertise include magnetic relaxation, transfer of angular momentum, spin fluctuations, spin-charge conversion, and exchange bias coupling.

He is familiar with supervisions at the master, doctoral and post-doctoral level, was the coordinator of several funded projects, contributed to several committees, is accustomed to organization of workshops and conferences, and authored several publications (71 including 1 RMP, 16 PRB, and 5 PRL, ~2000 citations).

EX-11-CLI04

Nanocrystalline formation of the iron-based soft magnet FINEMET studied by operando muon spin rotation technique

*[A. Koda](#)¹, C. Ohmori², Y. Yoshizawa², M. Ota³, K. Ogura³, D. Azuma³, N. Chiwata³, Y. Miyake¹

¹ Muon Science Laboratory, Institute of Materials and Structural Science, High Energy Accelerator Research Organization (KEK), Tokai, Naka, Ibaraki 319-1106, Japan

² Accelerator Laboratory, High Energy Accelerator Research Organization (KEK), Tokai, Naka, Ibaraki 319-1106, Japan

³ Hitachi Metals, Ltd., Minato-ku, Tokyo 108-8224, Japan

* coda@post.kek.jp

Keywords: FINEMET, soft magnetic material, nanocrystalline grain, operando measurement, μ SR

FINEMET® has prevailed in our daily life. It was discovered in 1988 by Yoshizawa *et al.* that nano-sized grains formed by heat treatment of Fe-Cu-Nb-Si-B amorphous alloy exhibit superior soft magnetic behavior. Because of the high permeability and the high saturating magnetization, as well as the quite small magnetostriction, FINEMET® becomes widely used in many electronic power devices in these days. Accelerator facilities are no exception. It is emphasized that J-PARC (Japan Proton Accelerator Research Complex) is a pioneer to utilize FINEMET® as the wideband RF cavity.

Besides the high functionality, the microscopic mechanism of the nanocrystalline formation under magnetic field is yet to be clarified. It is well-known that the magnetic properties are controlled by applying magnetic field during the heat treatment. This gives an idea that the magnetic entropy plays an important role on the nano-crystal growing. Muon is a local magnetic probe, which sensitively detects the formation of ferromagnetic nano-crystals in FINEMET®. Moreover, the world's highest pulsed muon beam in J-PARC provides us an opportunity of *in situ* observation of time-derived development of the magnetic grains. Since 2010, we have started studying the nanocrystalline formation of FINEMET® under magnetic field at elevated temperature by using operando muon spin rotation (μ SR) technique. The field-dependent behavior of nanocrystalline formation is reported.



- 1997 Doctor of Science, Osaka University
- 1999 Postdoctoral Fellow, Meson Science Laboratory, High Energy Accelerator Research Organization (KEK)
- 2002 Research Fellowship for Young Scientists, Japan Society for the Promotion of Science
- 2005 Research Associate, Muon Science Laboratory, High Energy Accelerator Research Organization (KEK)
- 2006 Muon Section, Materials and Life Science Division, J-PARC center
- 2019 Associate Professor, Muon Science Laboratory, High Energy Accelerator Research Organization (KEK)

FX-12-CLK01

Hard X-ray spectro-ptychography: Visualization of heterogeneous oxygen storage behavior in three-way catalyst particles

*Yukio Takahashi^{1,2,3}

¹Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, 980-8577, Japan

²Graduate School of Engineering, Osaka University, Suita, Osaka 565-0871, Japan

³RIKEN SPring-8 Center, Kouto, Sayo-cho, Sayo, Hyogo, 679-5148, Japan

*ytakahashi@tohoku.ac.jp

Keywords : X-ray spectro-ptychography, Oxygen storage, Three-way catalysts

X-ray ptychography is a rapidly emerging technique at synchrotron facilities, which can non-destructively observe thick samples at the nanoscale. So far, we have developed the techniques for high-resolution and high-sensitivity hard X-ray ptychography using total-reflection mirrors as the X-ray focusing device at SPring-8 in Japan [1,2]. The use of X-rays as a probe makes it possible to image both structures and chemical states through the absorption edges of a target element. X-ray ptychography using multiple energies including the absorption edge of a specific element, which is often referred to as X-ray spectro-ptychography, enables us to visualize the chemical state of nanostructures buried within thick samples. Hard X-ray spectro-ptychography (HXSP) is a promising tool for effectively and efficiently tackling the intrinsically complicated mesoscale materials science and chemistry.

Recently, we have demonstrated the two-dimensional(2D) visualization of the cerium valence in micrometer-size platinum-supported cerium-zirconium oxide Pt/Ce₂Zr₂O_x (x=7–8) three-way catalyst particles at better than 50 nm resolution by HXSP [3]. However, significant ambiguities, especially regarding the three-dimensional(3D) oxygen-diffusion-driven cerium oxidation tracking areas in individual Pt/Ce₂Zr₂O_x particles during the heterogeneous oxygen storage process, remain in the 2D images derived from projection of the structure and valence state along the optical axis. 3D HXSP combined with computed tomography can completely visualize the chemical states inside bulk materials, although the huge amount of structural and chemical data in real 3D space. Very recently, we have proposed the approach of 3D HXSP imaging coupled with unsupervised learning to achieve the 3D nanoscale chemical imaging of heterogeneous reaction events in bulk solid materials [4]. The 3D HXSP method allowed realization of 3D nanoscale imaging of the structure and valence state inside individual Pt/Ce₂Zr₂O_x particles during the oxygen storage process. Unsupervised data mining of the visualized 3D nanoscale chemical maps then successfully revealed the concealed heterogeneous oxygen-diffusion-driven 3D nanoscale Ce oxidation tracking areas inside the individual mixed-oxide particles during the oxygen storage process.

3D HXSP is expected to be an indispensable tool for determining the relationships between the structure and function of heterogeneous functional materials. In particular, in next-generation synchrotron facilities where fluxes with much higher coherence will be achieved, the present approach will be applied to in-situ 3D measurements, which can be expected to significantly accelerate progress in mesoscale materials science and chemistry.

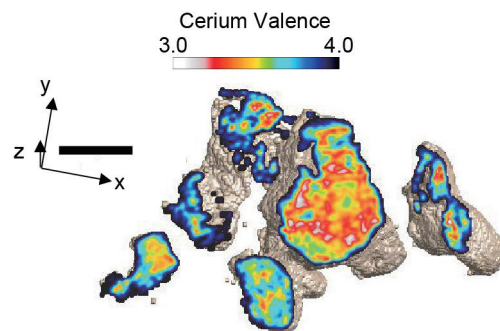


Fig. 1. 3D Ce valence image of Pt/Ce₂Zr₂O_x particles. The scale bar is 700 nm.

References

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Brief Personal History:

Yukio Takahashi is a professor at the Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University. His research interests lie in the development of new coherent X-ray imaging techniques for characterization of functional materials. He received his PhD degree in engineering from the Tohoku University in 2004. After a two-year postdoctoral researcher at the RIKEN SPring-8 Center, he became a lecturer at the Osaka University in 2007 and an associate professor in 2011. He became a professor at the Tohoku University in 2019.

FX-12-CLK02

Quantifying Inactive Lithium in Lithium Metal Batteries

*Y. S. Meng^{1,2}, C. Fang²

¹ Department of NanoEngineering, University of California San Diego, La Jolla, 92093, USA

² Materials Science and Engineering Program, University of California San Diego, La Jolla, 92093, USA

* shirleymeng@ucsd.edu

Keywords: lithium metal, inactive lithium, quantification, failure mechanism, mitigation strategies

Inactive lithium (Li) formation is the immediate cause of capacity loss and catastrophic failure of Li metal batteries. However, the chemical component and the atomic level structure of inactive Li have rarely been studied due to the lack of effective diagnosis tools to accurately differentiate Li^+ in solid electrolyte interphase (SEI) components and the electrically isolated unreacted metallic Li^0 , which together comprise the inactive Li. In this work, by establishing a new analytical method, Titration Gas Chromatography (TGC), we accurately quantify the contribution from unreacted metallic Li^0 to the total amount of inactive Li. We identify the Li^0 , rather than the Li^+ in SEI, as the dominating cause for the inactive Li and capacity loss. Using cryogenic electron microscopies to further reveal the micro- and nanostructure of inactive Li, we find that the Li^0 is

surrounded by insulating SEI, losing the electronic conductive pathway to the bulk electrode. Coupling the measurements of the Li^0 global content to

observations of its local atomic structure, we reveal the formation mechanism of inactive Li in different types of electrolytes, and identify the true underlying cause of low Coulombic efficiency in Li metal deposition and stripping. We ultimately propose strategies for highly efficient Li deposition and stripping to enable Li metal anode for next generation high energy batteries.

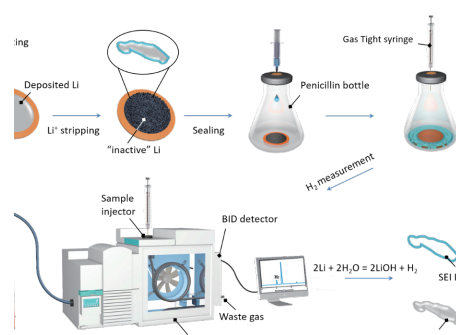


Fig. 1. Schematic working principle of the TGC method.

References:

1) C. Fang, Y.S. Meng* *et al*, Quantifying Inactive Lithium in Lithium Metal Batteries, Nature, accepted, 2019



Dr. Y. Shirley Meng

Zable Endowed Chair Professor in Energy Technologies
BA in Materials Engineering from Nanyang Technology University in 2000.

Ph.D. in Advance Materials for Micro & Nano Systems from the Singapore-MIT Alliance in 2005.

Postdoct Fellow and Research Scientist at MIT 2005-2008

Assistant Professor, Materials Science and Engineering, University of Florida in 2009

Assistant Professor (2009-2013), Associate Professor (2013-2017) and Full Professor (2017 – present) at NanoEngineering, University of California, San Diego

Principal Investigator of Laboratory for Energy Storage and Conversion, <http://smeng.ucsd.edu/>

shirleymeng@ucsd.edu

PROFESSIONAL MEMBERSHIP/AWARDS

- Founding Director of Sustainable Power and Energy Center, <http://spec.ucsd.edu/>
- Serve as Executive Board Member and Secretary (Elected) for Battery Division of the Electrochemical Society USA (2014 – present)
- Serve as the Executive Board Member and Treasurer for International Battery Association (IBA) (2017 – present)
- Fellow of the Electrochemical Society (2018 – present)
- Faculty Excellence Award in Research in Science and Engineering (2019)
- International Battery Materials Association IBA2019 Research Award (2019)
- IUMRS-Singapore Young Scientist Research Award (2017)

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GX-13-CLK01

Soft Electronic and Robotic Systems

*Martin Kaltenbrunner^{1,2}

¹ Department of Soft Matter Physics, Johannes Kepler University Linz, Altenbergerstr. 69, 4040 Linz, Austria

² Soft Materials Laboratory, Linz Institute of Technology, Johannes Kepler University Linz, Altenbergerstr. 69, 4040 Linz, Austria

* martin.kaltenbrunner@jku.at

Keywords: Soft Electronics, Soft Robotics, Electronic Skins, Biodegradable materials, Tough Hydrogels, Stretchable Electronics, Soft Sensors

Electronics of tomorrow will be imperceptible and will form a seamless link between soft, living beings and the digital world. Exploring the fundamental physics, mechanical form factors, and materials required to meet the needs of this new generation of *soft* electronics and *soft* machines is driving multidisciplinary research worldwide. Weight, flexibility and conformability are pivotal for future wearable, soft and stretchable electronics to proliferate. The abilities to be imperceptible, epidermal, transient and self-healing are fueling the vision of autonomous smart appliances to be embedded everywhere, on textiles, on our skin, and even in our body.

This talk introduces a technology platform for the development of large-area, ultrathin and lightweight electronic and photonic devices, including solar cells, light emitting diodes and photodetectors, active-matrix touch panels, implantable organic electronics, imperceptible electronic wraps and “sixth-sense” magnetoception in electronic skins. Air stable perovskite solar cells, only 3 μm thick, endure extreme mechanical deformation and have an unprecedented power output per weight of 23 W/g. Highly flexible, stretchable organic light emitting diodes are combined with photodetectors for on-skin photonics and pulse oximetry, providing electrical functionality in yet unexplored ways. Tactile sensor arrays based on active-matrix organic thin film transistors can be operated at elevated temperatures and in aqueous environments as an imperceptible sensing system that ensures the smallest possible discomfort for patients requiring medical care and monitoring. Combined with organic amplifiers and biocompatible conductive gels, we demonstrate *in vivo* recording of vital signals. E-skins with GMR-based magnetic field sensors equip the wearer with an unfamiliar sense that enables perceiving of and navigating in magnetic fields. These large area sensor networks build the framework for electronic foils and artificial sensor skins that are not only highly flexible but become highly stretchable and deployable when combined with engineered soft substrates such as elastomers, shape memory polymers or hydrogels. We show mobile health monitoring systems, smart, tissue-like electronics and soft robots that utilize tough hydrogels as soft transducers, generators and adaptive lenses. A newly developed direct writing method for ultrathin oxide dielectrics and semiconductors will allow low-cost and large area fabrication of such soft systems.

Tackling issues of sustainability and resourceful production, we here introduce materials and methods for soft systems that facilitate a broad range of applications, from transient wearable electronics to metabolizable soft robots. These embodiments are reversibly stretchable, are able to heal and are resistant to dehydration. Our forms of soft electronics and robots – built from resilient biogels with tunable mechanical properties – are designed for prolonged operation in ambient conditions without fatigue, but fully degrade after use through biological triggers. Electronic skins merged with imperceptible foil technologies provide sensory feedback such as pressure, strain, temperature and humidity sensing in combination with untethered data processing and communication through a recyclable on-board computation unit. Such advances in the synthesis of biodegradable, mechanically tough and stable iono- and hydrogels may bring bionic soft systems a step closer to nature.



Martin Kaltenbrunner
Soft Matter Physics Department,
LIT Soft Materials Lab,
Johannes Kepler University,
Altenberger Straße 69, 4040 Linz Austria;
Phone: +43 732 2468 9764
email martin.kaltenbrunner@jku.at.

Kaltenbrunner is a full professor at the Johannes Kepler University, heading the Soft Matter Physics Department and the LIT Soft Materials Lab. He received his master's and PhD degrees in physics from the Johannes Kepler University in 2008 and 2012, respectively. He then joined the Someya-Sekitani Lab for Organic Electronics at The University of Tokyo as postdoctoral researcher prior to his present position. Kaltenbrunner's research interests include soft electronics and machines, biodegradable soft materials, photovoltaics, lightning and thin film transistors, soft transducers and robotics, flexible and stretchable electronics, and electronic skin.

GX-13-CLK02

Design, development, and doping of novel inorganic optoelectronic functional materials

*Toshio Kamiya^{1,2}, and Hideo Hosono^{1,2}

¹Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan, ² Materials Research Center for Element Strategy, Tokyo Institute of Technology 4259 Nagatsuta, Midori-ku, Yokohama, 226-8503, Japan

* kamiya.t.aa@m.titech.ac.jp

Keywords: Optoelectronic devices, Materials design, Doping, Defects, Density functional theory

Many functional oxide materials are already used for active components of optoelectronic / mechanical devices such as piezoelectric actuators / gyroscopes, non-volatile memories such as ferroelectric RAM, positive temperature coefficient (PTC) thermistors, electrochromic anti-dazzle mirrors and so on. As for thin-film transistors (TFTs), the first proposal was given with CdS in 1961 by following the proposal of Si MOS field-effect transistors (FETs) in 1960. History of oxide FETs goes back also to mid 60's with SnO₂, In₂O₃ and ZnO FETs. However, the oxide TFT research had disappeared from open-accessible literatures after that, due probably to their instability. After the long incubation period, revival of oxide TFT research came up in 1996 as SnO₂ FET, and poly ZnO TFT has attracted intensive interest for overtaking the a-Si TFT technology. On the other hand, as known, e.g., in poly-Si TFTs, carrier transport, and device performances, and their stability are affected seriously by grain boundary issues in polycrystalline semiconductors. Amorphous oxide semiconductors (AOSs) represented by a-In-Ga-Zn-O (a-IGZO) then gathered practical interest due to their advantages over polycrystalline semiconductors; i.e., they are free from the grain boundary issues, their devices are fabricated at low temperature even at room temperature on glass / plastic substrate as well as they possess satisfactory high electron mobilities >10 cm²/(Vs); thus, they are now employed in many flat-panel displays from very high-resolution liquid-crystal displays to jumbo (up to 88 inch diagonal) organic light-emitting diode TVs. Although they are already commercialized, there remain many issues on their stability, and these are related closely to defects. Also for crystalline semiconductors, carrier doping is essential to develop new semiconductor materials and devices, while doping capability is often inactivated by so-called 'self-compensation' effects in particular for wide bandgap materials such as oxides and nitrides; therefore, understanding and control of such defects are critical to design and develop new functional materials.

In this paper, we will discuss what we need to consider to design and develop new functional materials with assistance of first-principles density functional theory (DFT) calculations. It will cover several categories of materials such as AOSs, ultrawide band gap materials, semiconductors, light-emitting materials, and thermoelectric materials, and also refer to the applications of DFT to extrapolating new materials, synthesizing high-quality materials with less defects, designing effective doping routes etc.



Toshio Kamiya started his research career as an assistant professor of Department of Inorganic Materials at Tokyo Tech., Tokyo, Japan, in 1991, and moved to Interdisciplinary Graduate School of Science and Engineering in 1996. He received the Dr(Eng) degree in materials science from Tokyo Institute of Technology in 1996. He spent two years at Microelectronics Research Centre, Cavendish Laboratory at the University of Cambridge as a visiting scholar from 2000 to 2002. He became an associate professor in 2002 and a full professor in 2010 in the Materials and Structures Laboratory at Tokyo Institute of Technology. He became the vice director of Materials Research Center for Element Strategy in 2012, and the director of Laboratory for Materials and Structures & vice director of Institute of Innovative Research in 2017.

His field of research includes exploration, materials design, and device applications of new functional inorganic materials. He has published about 400 scientific papers. He was awarded with The Ceramics Grand Prize by The Ceramics Society of Japan in 2016, SID Special Recognition Award in 2015, The CerSJ Awards for academic achievements in ceramic science and technology in 2013, Tejima Research Award (Invention) in 2011, The Young Scientists' Prize by MEXT in 2007, The Advanced Technology Award by the Fuji-Sankei group in 2005, etc, and the Fellow of The Japan Society of Applied Physics and The Ceramic Society of Japan.

Education

- April, 1986 – March, 1990: Undergraduate course at Department of Inorganic Materials, Faculty of Engineering, Tokyo Institute of Technology (Bachelor of Engineering)
- April, 1991 – March, 1992: Master Course at Department of Inorganic Materials, Graduate School of Engineering, Tokyo Institute of Technology
- March, 1992: Leave Department of Inorganic Materials, Tokyo Institute of Technology
- December, 1996: Obtain Doctor of Engineering at Department of Inorganic Materials, Tokyo Institute of Technology for Study on Dielectric Crystals by First-Principles and Molecular Simulations

Professional Appointments

- April, 1992: Assistant Professor of Department of Inorganic Materials, Tokyo Institute of Technology
- November, 1996: Move to Department of Electrochemistry, Interdisciplinary Graduate School of Science and Engineering, Tokyo Institute of Technology
- April, 1997: Move to Materials and Structures Laboratory, Tokyo Institute of Technology
- January, 2002: Lecturer at Materials and Structures Laboratory, Tokyo Institute of Technology
- December, 2003: Associate Professor at Materials and Structures Laboratory, Tokyo Institute of Technology
- August, 2010 – present: Professor at Materials and Structures Laboratory, Tokyo Institute of Technology
- July, 2012 – present: Vice Director of Materials Research Center for Element Strategy, Tokyo Institute of Technology
- July, 2017 – present: Vice Director of Institute of Innovative Research, Tokyo Institute of Technology
- July, 2017 – present: Director of Laboratory for Materials and Structures, Tokyo Institute of Technology

GX-13-CLK03

Gold Nanorods with Ultranarrow LSPR Bands

*Luis M. Liz-Marzán^{1,2}

¹ CIC biomaGUNE, Donostia-San Sebastián, 20014, Spain, ² Ikerbasque, Bilbao, 48003, Spain

* lizmarzan@cicbiomagune.es

Keywords: gold nanorods, seeded growth, localized surface plasmon resonance, ultrafast lasers

Although seeded-growth methods have made available to us an extensive library of anisotropic metal nanoparticles, the chemical complexity of the growth solution, often involving organic additives, and the structural instability of the seeds hinder the quest for high quality products. For the sake of synthetic simplicity, merging different synthetic protocols by finding common growth routes, is a mandatory step to reach a universal growth mechanism and reproducible fabrication. This communication will introduce two recent discoveries, related to improving the optical quality of both pentatwinned and single crystal gold nanorods.

We recently demonstrated that a thermal treatment of small seeds results in extensive twinning and a subsequent drastic yield improvement (>85%) in the formation of different types of pentatwinned nanoparticles, including nanorods, with a high monodispersity and tunable aspect ratio.

On the other hand, although single crystal Au nanorods can be readily obtained with very high quality directly from optimized seeded growth methods, polydispersities below 10% are still difficult to reach, which leads to some broadening of the longitudinal LSPR band. We show here that femtosecond laser irradiation may lead to significant narrowing of the LSPR band, even to the limit of the single particle, as calculated from theoretical models, meaning pure “optical monodispersity”.

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Luis Liz-Marzán is Ikerbasque Professor and Scientific Director of the Center for Cooperative Research in Biomaterials, CIC biomaGUNE, in San Sebastián (Spain), since September 2012. He graduated in chemistry from the University of Santiago de Compostela, was postdoc at Utrecht University and Professor at the University of Vigo, Spain (1995–2012). He has been Invited Professor at Tohoku University, University of Michigan, University of Melbourne, University of Hamburg, the Max-Planck Institute of Colloids and Interfaces, King Saud University, Ecole Normale Supérieure Paris-Saclay and Jiangnan University. Liz-Marzán received numerous research awards, including a Humboldt research award, ACS Nano lecture award, Langmuir lectureship, Rhodia Prize of the European Colloid and Interface Society, Medal of the Spanish Royal Society of Chemistry, Rey Jaime I award, National Chemistry Prize of Spain, as well as 2 ERC Advanced Grants. He is also member of the Royal Spanish Academy of Sciences, the European Academy of Sciences and Academia Europaea. He is a highly cited researcher who has co-authored over 450 publications and 8 patents, and has delivered over 450 invited lectures and seminars worldwide. Liz-Marzán has supervised over 30 PhD students and 50 postdocs, many of them holding academic positions worldwide. He is currently associate editor of ACS Nano, has been senior editor of Langmuir and co-editor of ACS Omega, and serves in the editorial boards of various other journals, including Science. His major research activity is devoted to understand the growth mechanisms of metal nanocrystals, to tailor their surface chemistry and thereby directing their self-assembly. He also works on the design of biomedical applications based on the plasmonic properties of well-defined metal nanoparticles and nanostructures, including surface enhanced Raman scattering.

GX-13-CLK04

Perovskite Solar Cells: History, Progress and Perspective

*Nam-Gyu Park

School of Chemical Engineering, Sungkyunkwan University (SKKU), Suwon 16419, Korea

* npark@skku.edu

Keywords: Perovskite, Solar Cell, High Efficiency, Large-area

Since the first report on the 9.7% efficiency, 500 h-stable solid-state perovskite solar cell (PSC) in 2012 by our group, following two seed works on perovskite-sensitized liquid junction solar cells in 2009 (Miyasaka et al) and 2011 (Park et al), a power conversion efficiency (PCE) of 25.2% was recorded in 2019. According to Web of Science, publications on PSC increase exponentially since 2012 and total number of publications reaches over 13,000 as of August 2019, which indicates that PSC is considered as promising photovoltaics.

Although high photovoltaic performance was achieved from small area cell, scalable technologies are required for commercialization of PSC. In order to shift from small-area device to large-area module, the cheap materials and an effective coating procedure are highly required. We developed cost-effective materials based on delta FAPbI₃ powder for high efficiency PSC. The best PCE of 22.6% was achieved using the synthesized perovskite powder (certified stabilized efficiency was 21%). For large-area uniform perovskite coating, a precursor solution containing perovskite cluster was developed. Homogeneous MAPbI₃ perovskite film (>100 cm²) was D-bar coated within 20 s, which demonstrated the PCE approaching 18%. Bifacial stamping technique was developed, which led to both high quality FAPbI₃ and MAPbI₃ on a large scale at milder condition. For higher efficiency, managing interfacial recombination is of critical importance. Interfacial engineering with organic or inorganic materials is found to improve voltage and fill factor, confirming that reduction in recombination can result in improvement of photovoltaic performance of PSC.

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Nam-Gyu Park is Distinguished professor and SKKU-Fellow at School of Chemical Engineering, Sungkyunkwan University (SKKU). He received his B.S. degree in chemical education, M.S. and Ph.D. degrees in chemistry from Seoul National University in 1988, 1992 and 1995, respectively. He worked at ICMCB-CNRS, France, from 1996 to 1997 and at National Renewable Energy Laboratory, USA, from 1997 to 1999 as postdoctoral researchers. He was director of solar cell research center at Korea Institute of Science and Technology (KIST) from 2005 to 2009 and principal scientist at Electronics and Telecommunications Research Institute (ETRI) from 2000 to 2005 before joining SKKU as a full professor in 2009. He is a fellow of Korean Academy of Science and Technology (KAST) since 2017. He has been working on high efficiency mesoscopic nanostructured solar cells since 1997. *He is pioneer of solid-state perovskite solar cell, which was first developed in 2012.* He was selected as a *New*

Class of Nobel Prize-Worthy Scientists in September 20, 2017 and included in *highly cited researchers (top 1% scientists)* in Nov. 15, 2017 and Nov. 27, 2018 by Clarivate Analytics. He received awards including Scientist Award of the Month (2008), KIST Award of the Year (2009), Dupont Science and Technology Award (2010), SKKU fellowship (2013 and 2018), PVSEC Hamakawa Award (2015), Dukmyung KAST Engineering Award (2016), ACS-KCS Excellence Award (2018), and Samsung *Ho-Am Prize* (2018). Prof. Park has currently more than 300 refereed publications and more than 70 patents. He received H-index of 84 (google scholar). He is senior Editor of ACS Energy Letters and serves on the Editorial Advisory Board for Chem. Rev., ChemSusChem, and Solar RRL.

HX-11-CLK01

Photocatalytic water splitting for solar hydrogen production

*Kazunari Domen^{1,2}

¹ Research Initiative for Supra-Materials, Shinshu University, Nagano-shi, Nagano 380-8553, Japan, ² The University of Tokyo, Bunkyo-ku, Tokyo 113-8656, Japan

*domen@shinshu-u.ac.jp; domen@chemsys.t.u-tokyo.ac.jp

Keywords: Particulate photocatalyst, Photocatalyst sheet, Panel reactor, Scalability, Non-oxide, Cocatalyst

Sunlight-driven water splitting has been studied actively for production of renewable solar hydrogen as a storable and transportable energy carrier.¹⁾ Both the efficiency and the scalability of water-splitting systems are essential factors for practical utilization of renewable solar hydrogen. Particulate photocatalyst systems do not involve any secure electric circuit and can be spread over wide areas by inexpensive processes potentially. It is therefore important to activate particulate photocatalysts and develop their reaction systems.

SrTiO₃ is a photocatalyst active in overall water splitting under UV light irradiation with loading of proper cocatalysts. The author's group has found that doping Al into SrTiO₃ boosts the water splitting activity by two orders of magnitude.²⁾ Through tuning of the preparation and modification methods of Al-doped SrTiO₃, the apparent quantum yield of photocatalytic water splitting has been upgraded to 56% and even greater at 365 nm. Panel reactors are studied to spread such active particulate photocatalysts (Fig. 1). Particulate photocatalysts are thinly fixed on substrates, and such “photocatalyst sheets” are contained in panel reactors. A panel reactor containing Al-doped SrTiO₃ photocatalyst sheets releases product hydrogen and oxygen gas bubbles at a rate corresponding to a solar-to-hydrogen energy conversion efficiency of 10% under intense UV illumination even when the water depth is merely 1 mm, and it can maintain the activity over several months under sunlight illumination.³⁾ A 1-m²-sized photocatalyst panel reactor splits water under natural sunlight irradiation without a significant loss of the intrinsic activity of the photocatalyst sheets.²⁾ Panel-type reactors can accommodate various kinds of photocatalysts sheets and are expected to be built using light and inexpensive materials, being suitable for large-scale solar hydrogen production from water.

In practice, it is essential to develop photocatalysts active under visible light irradiation. Various oxides, (oxy)nitrides, and (oxy)chalcogenides have been developed.⁴⁾ Some non-oxide photocatalysts can split water into hydrogen and oxygen under irradiation of up to approximately 600 nm. Two different photocatalysts can also be combined so that hydrogen and oxygen are evolved on the respective photocatalysts efficiently.

In my talk, the latest progress in photocatalytic materials and reactors and concepts toward large-scale demonstration will be presented.

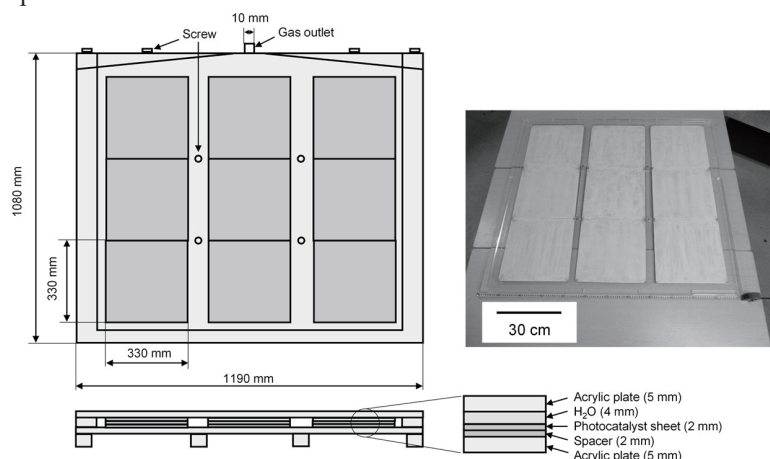


Fig. 1. A 1-m²-sized photocatalyst panel reactor accommodating photocatalyst sheets. Reprinted with permission from ref. 2. Copyright © 2017 Elsevier Inc.

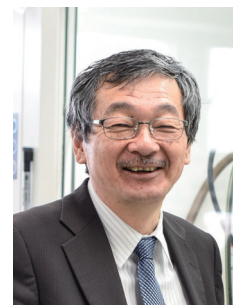
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Curriculum Vitae:

Name: Kazunari DOMEN

- Special Contract Professor, Research Initiative for Supra-Materials (RISM), Shinshu University
- University Professor, The University of Tokyo



Research interests:

- Development of photocatalysts for water splitting and solar hydrogen production
- Study on reaction mechanisms of heterogeneous catalysis by Infrared Spectroscopy
- Surface reaction dynamics by nonlinear laser spectroscopy
- Development of new functional materials for catalysis

Academic Background:

- 1976 B.S. The University of Tokyo
- 1979 M.S. The University of Tokyo, School of Science
- 1982 Ph.D. The University of Tokyo, School of Science

Professional Career:

- 1982-1990 Associate Researchers, Chemical Resources Laboratory, Tokyo Institute of Technology
- 1990-1996 Associate Professor, Chemical Resources Laboratory, Tokyo Institute of Technology
- 1996-2004 Professor, Chemical Resources Laboratory, Tokyo Institute of Technology
- 2004-2019 Professor, Department of Chemical System Engineering, School of Engineering, The University of Tokyo
- (Visiting Scientist at IBM Almaden Research Center from 1985 to 1986.)
- 2017-present Special Contract Professor, Cross appointment, Center for Energy & Environmental Science, Shinshu University
- 2019-present Special Contract Professor of Research Initiative for Supra-Materials (RISM), Shinshu University
- 2019-present University Professor, the University of Tokyo

Awards & Honors:

- 1990; Encouragement Prize, Catalysis Society of Japan,
- 1991; Catalyst Preparation Awards,
- 2007; Catalysis Society of Japan Awards
- 2011; The Chemical Society of Japan Awards
- 2018; The Japan Petroleum Institute Award
- 2018; The Japanese Photochemistry Association Lectureship Award
- 2019; Lee Hsun Lecture Award
- 2019; Advance of Catalysis Award of APACS

HX-11-CLK02

Plasma Synthesis, Conversion, and Processing of Energetic Materials

*[Alexander Fridman](#)

Drexel University, Nyheim Plasma Institute, Philadelphia, Pennsylvania, USA, 19104)

*fridman@drexel.edu

Keywords: gliding arcs, pulsed plasma, methane conversion, polymeric nitrogen

Presentation reviews latest experimental results obtained in Nyheim Plasma Institute of Drexel University on plasma-chemical material treatment processes, focused on liquid and gas fuel conversion and processing, as well as on plasma-chemical synthesis of novel energetic materials in non-thermal plasma discharges. Major discharges in focus are:

1. *Non-equilibrium gliding arcs stabilized in reverse vortex Tornado flow:*

Physics and plasma parameters of gliding arcs will be discussed in relation to their material processing abilities and effectiveness

2. *Micro- and nanosecond pulsed dielectric barrier discharges*

Physics and plasma parameters of pulsed DBD in gases and liquids will be discussed in relation to their material processing abilities and effectiveness

3. *Cold and transitional discharges in liquids*

Physics and plasma parameters of cold discharges in liquids without bubbles will be discussed in relation to their material processing abilities and effectiveness

Major specific plasma-chemical processes in focus are:

1. Methane conversion in mixture with different gases
2. Methane (natural gas) direct liquefaction process
3. Liquid-phase synthesis of polymeric nitrogen compounds

Mechanisms of the plasma-chemical processes and produced materials characterization are discussed in this presentation, as well as physical and plasma-chemical kinetics of the processes in strongly non-equilibrium conditions

Alexander Fridman received the B.S./M.S. and Ph.D. degrees in physics and mathematics from the Moscow Institute of Physics and Technology, Moscow, Russia, in 1976 and 1979, respectively, and the D.Sc. degree in mathematics from the Kurchatov Institute of Atomic Energy, Moscow, in 1987. He is the Nyheim Chair Professor of Drexel University, Philadelphia, PA, and the Director of the Drexel Plasma Institute, where he works on plasma approaches to material treatment, fuel conversion, and environmental control. He has more than 30 years of plasma research experience in national laboratories and universities of Russia, France, and USA. He has authored or coauthored five books and more than 350 papers. Prof. Fridman was a recipient of numerous awards, including the Stanley Kaplan Distinguished Professorship in Chemical Kinetics and Energy Systems, the George Soros Distinguished Professorship in Physics, and the State Prize of the U.S.S.R. for the discovery of selective stimulation of chemical processes in nonthermal plasma, ICRP Award, and Plasma Chemistry Award.



HX-11-CLK03

Gallia(Ga₂O₃) for Green and Efficient Energy applications

* E.Chikoidze¹, A.Perez-Tomas², C.Sartel¹, D. J. Rogers³, C. Y .Dumont¹

¹ Université de Versailles- CNRS, Université Paris-Saclay, Versailles, 78035, France

²Catalan Institute of Nanoscience and Nanotechnology (ICN2), Barcelona, 08010, Spain

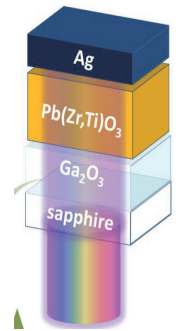
³Nanovation, Châteaufort, 78117 France

*Ekaterine.chikoidze@uvsq.fr

Keywords : Gallium Oxide, Optoelectronic properties; Solar and Power Electronics;

Renewable **Solar energy** is becoming a mainstream source of energy, and **power electronics** is a key enabler of its' successful integration. Recent breakthroughs in material quality have led to a “rediscovery” of Ga₂O₃ such as a high band gap (~5eV) transparent conductor, transparent field-effect transistors, photodetectors but also as a platform for power electronic devices.

An unexpectedly low 2D-like resistivity has been shown for n type Ga₂O₃/r-Al₂O₃ which is resistant to high dose proton irradiation and largely invariant (metallic) over temperatures from 2 to 850K.¹ The remarkable resilience and stability of the electrical properties under thermal and highly ionizing radiation stressing, combined with the extended transparency range and the known toughness under high electrical field could open up new perspectives for use as expanded spectral range transparent electrodes (e.g. for UV harvesting solar cells or UV LEDs/lasers) as well as robust Ohmic contacts for use in extreme environments/applications. As an example, we have showed the use of Ga₂O₃ electrodes has enabled, for the first time, an above-bandgap bulk photovoltaic effect on sandwich-like capacitors with transparent conducting electrodes (the architecture of solar cells) and under white light. These are crucial



breakthroughs towards the implementation of the bulk photovoltaic effect in solar cells.² Fig. 1. Schematic of the sandwiched structure of the archetypical thin-film solar cell;

While there are several *n*-type transparent semiconductor oxides (TSO) for optoelectronic applications their required *p*-type counterparts oxides are known to be more challenging. We have demonstrated that Ga₂O₃ is also the intrinsic (or native) *p*-type TSO³ with the largest bandgap for any reported *p*-type TSO (e.g. NiO, SnO, delafossites, oxychalcogenides). The achievement of hole mobility in excess of 10 cm²/Vs and (high temperature) free hole concentrations in the ~10¹⁷ cm⁻³ range.⁴ Fig.2

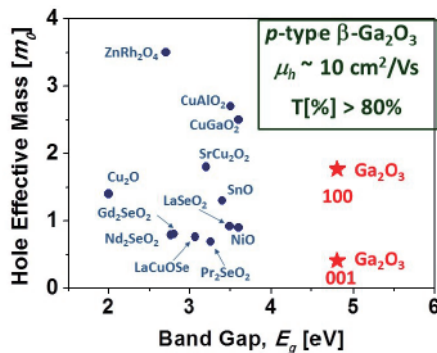


Fig.2 Hole Effective masses for different oxides. Insert: results for Ga₂O₃ from our experiment

Attaining p-type doping in gallium oxide may already be an important step for technological integration. Mainly, in power applications, the p-type demonstration is particularly important as the p-n junction could sustain larger voltages than any Schottky unipolar junction. In other words, the demonstration of Ga₂O₃ bipolarity represents a definitive step forward when considering this potentially low-cost oxide wide band gap semiconductor technology in power applications now dominated by the prohibitively expensive Silicon Carbide substrates.

Surprising optoelectronic properties of Gallia opens a new pathway for “Oxitronics” integration in Renewable energy technologies and electrical vehicles.

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Ekaterine Chikoidze 1992 Graduated with honour Faculty of Physics, Material Science Department at Tbilisi State University, Georgia; 1992- 1995 working as a translator (Russian, Italian, English) in editorial houses of journals /newspapers. 1996-1999 Doctorate student Material Science Department at Tbilisi State University, Georgia; 1999 PhD in the field of “semiconductors and dielectrics”.From 2000-2006 Senior researcher in the lab of semiconductor material science. 2001-2003 Visiting Researcher in Politecnico di Milano, Department of Physics, centre of Ultrafast phenomenon and Biomedical Optics Optics, Italy. 2003–2006 Visiting Researcher in CNRS, France. 2007-present permanent researcher and scientific communication manager of the laboratory GEMaC, CNRS, Paris Saclay University, France. Coordinator of several bilateral, national and international projects, member of EU networks, Organizer of several workshops and member of scientific committees.

Having more than 20 years of experience of working in the field of physical properties of Wide band gap materials : ZnS, Diamond, ZnO, 3d magnetic oxides, Cu based transparent conducting oxides, Gallium Oxide. The one of the main focus activity is build up the specific instrumentation and study electrical and magneto transport properties of Oxides. In GEMaC/CNRS she has developed several home built experimental instrumentation dedicated to study highly resistive thin films: Seebeck Effect, Photoconductivity upgraded PPMS(Quantum design) set up, giving possibility to measure extremely high (up to 100GOhm) resistive materials in a very broad range of temperature and magnetic field. Having collaborations with researchers from 12 countries, author of 68 publications, 89 participations in Conferences, 10 invited talks.

Research Gate:https://www.researchgate.net/profile/E_Chikoidze

HX-11-CLK04

Lead-free Piezoelectric Ceramics - Future perspectives -

* Akira Ando

Murata Manufacturing Co., Ltd.

* a_ando@murata.com

Keywords: Piezoelectric PZT lead-free sensor, actuator

Various lead free piezoelectric material families such as alkaline niobates, bismuth perovskites, bismuth layer structured ferroelectrics (BLSF) etc. have been researched for long time more than 60 years.

These lead free materials were almost discovered in the USA in processes of pursuing good piezoelectric materials for telecommunication devices in 1950's¹⁾. However, after the discovery of Pb(Ti, Zr)O₃ (PZT) family materials with high piezoelectric characteristics, the above researches on the lead free piezoelectric materials soon decreased.

Public concern for environmental pollution raised in 1970's, then researches on the lead free piezoelectric materials became active again in the USA and in Japan¹⁾. Basic data of characteristics of the lead free piezoelectric materials were taken at this time, however no lead free materials could not exceed the PZT, the researches on the lead free materials decreased.

Importance of Environments CONscious (ECO) technologies was widely recognized again in 1990's and the researches on lead free piezoelectric materials have become active again.

At this time, several lead free materials which partly exceed PZTs were discovered.

For example, some BLSF materials are better than PZTs as resonator materials²⁾, and Bi perovskites show better ultrasonic vibration characteristics than those of PZTs³⁾.

Furthermore, practical non-oxide piezoelectric materials; Sc doped AlN were developed in Japan for thin film resonator devices⁴⁾, and they have already made huge industries in the USA.

In the presentation these histories of researches on various lead free piezoelectric material are reviewed, and their current status and future perspectives are described.

References (Example: non-mandatory, 10 point):

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Biography

Dr. Akira Ando is a general manager of material development department of Murata Mfg. Co., Ltd. He has joined Murata Mfg. Co., Ltd. soon after he graduated from Hiroshima University in 1983. He received doctoral degree from Tokyo Institute of Technology at 2003. He is in charge of research and development in new material technologies. His expertise is research and development on functional ceramics such as piezoelectric or other ferroelectric materials and applications. He received the Richard Fulrath award from the American ceramic society (2002), and the academic award from the ceramic society of Japan (2009).



IX-13-CLK01

Importance of strengthening “venous industry” for future plastics

*N. Kawashima

Shiodome City Center, 1-5-2, Higashi Shimbashi, Minato-ku, Tokyo 105-7122, Japan

*Nobuyuki.kawashima@mitsuichemicals.com

Keywords: Fossil-based plastics, Bioplastics, Circular Economy, Venous Industry

Plastics contribute to healthy and sound everyday life, but the chemical industry is facing new challenges from the viewpoints of resource depletion and environmental burden. Now is the time to explore the future direction of plastics. Merely pursuing cost and performance improvements of materials will not solve impending social, waste management, and environmental issues. A holistic approach, which includes raw material



Fig. 1. Resilient and sustainable economic growth requires an integrated scheme among resource circulation, carbon neutrality, and social systems. This figure was prepared by the author (Kawashima).

conversion and efficient after-use treatment, is necessary. Additionally, resource circulation alone will not realize resilient and sustainable economic growth. Instead a Circular Economy, which was initially suggested in Europe and involves resource circulation such as

maintenance, repair, and reuse/recycle, should be expressed by an integrated scheme among resource circulation, carbon neutrality, and social systems (Fig. 1). This transition will be accelerated by digitalization and knowledge sharing such as artificial intelligence and robotics.

Figure 2 shows a plastics circulation model. Current plastics circulation tends to focus on resource circulation. However, the era of business models only considering materials is over. Future fossil-based plastics and bioplastics models must encompass raw materials, plastic products, applications, and waste management.

After utilization of fossil-based plastics, circulation will not be feasible if the collection and sorting quality is insufficient or economically unsustainable. Similarly, circulation of bioplastics will not be realized if biomass prices become higher or the dependency on edible resources increases. Even with recycling, a resilient, robust, and sustainable business will not be achieved unless an economical competitive business model is constructed considering the three elements described in Fig. 1. How can a circular economy model for plastics be strengthened? One way is to introduce new perspectives such as digital technologies and collaborating with other industries such as agriculture and CCUS.

A circular plastics economy is analogous to blood vessels in which linear flows from raw materials to products (Fig. 2, black lines) correspond to arteries, and circular arcs from products to various circulations (blue and green lines) correspond to veins. The future direction for plastics should include a circulating value chain. Similar to the harmonious relationship between arteries and veins in blood vessels, the venous industry should be strengthened in order to provide value to be sufficiently linked to the arterial industry.

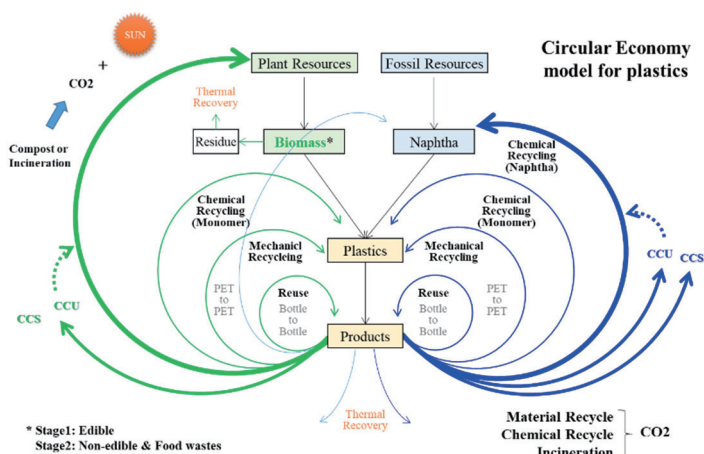


Fig. 2. Circular economy for plastics, including both fossil-based plastics and bioplastics. This figure was prepared by the author (Kawashima).

Reference:

1) N. Kawashima, T. Yagi, K. Kojima, *Macromolecular Materials and Engineering* 1900383 (2019). <https://doi.org/10.1002/mame.201900383>

Curriculum Vitae

Nobuyuki Kawashima holds a Masters' degree from the School of Science, Osaka University where he majored in organic chemistry. After joining Mitsui Chemicals in 1979, he worked in biochemistry and molecular biology at the Central Research Lab and the City of Hope National Medical Center in California. From 1990–2009, he focused on new business developments, including polylactic acid. He served as the Executive Director and the Secretary General of the Chemical Society of Japan from 2009–2016. Currently, he is the Chair of Energy and Climate Change Leadership Group, ICCA.



IX-13-CLK02

Ceramic Additive Manufacturing Technologies for Biomedical applications

*Hui-suk Yun^{1,2}

¹ Korea Institute of Materials Science (KIMS), Changwon, 51508, Republic of Korea, ² University of Science & Technology (UST), Changwon, 51508, Republic of Korea

* yuni@kims.re.kr

Keywords: Additive manufacturing, 3D printing, Stereolithography, Material Extruding, Ceramics, Biomedical

3D printing, also called additive manufacturing (AM), is a fabrication process that used digital information from a computer-aided design file to stack 2D layers of various materials to produce a 3D object, without requiring any part-specific tooling. AM technologies have attracted much attention in various fields such as biomedical industry, automotive, aerospace, consumer, and other industrial application. AM technology especially offers significant advantages in the medical industry as it permits the on-demand manufacture of low-volume or one-of-a-kind parts based on patient-specific needs. AM in the medical industry, both actual and potential, can be organized into several broad categories, including tissue and organ fabrication, customized prosthetics, implants, anatomical models, and pharmaceuticals.

Synthetic materials that are clinically favored for bone tissue regeneration are mainly those based on bioceramics due to the chemical similarity of bioceramics to the mineral phase of bone. Nevertheless, the development of ceramics AM technology has been very slow when compared with other materials, due largely to the difficulty and complexity of the fabrication process, i.e. ceramics generally require both debinding and sintering steps after printing, which can lead to deformation and unstable mechanical properties of the printed 3D structure. However, successful cases for commercialization have been reported recently, and several new technologies now appear to overcome the limitations of ceramics AM.

Our group has developed a novel stereolithography based AM system, which has been designed specifically to overcome the complications of typical vat-type stereolithography system. The fabrication system and processing has been successfully optimized for various types of materials for fine control over the end product. We could co-print multi-component in one structure using less amount of ceramic slurry with high resource efficiency. We have confirmed multi-material printability of both the functionally graded material (FGM) structures and the core-shell structure. We can expect various applications of our new technology in medical fields. For example, possibility of producing FGM structure using AM technique will make us possible to fabricate custom-made dental crown which can design not only controlling shape but also adjusting both color gradation and transparency. Possibility of fabricating core-shell structure will provide a chance to us for designing multi-functional medical device. Our group also has suggested unique ceramic AM process for creation of bioceramic scaffolds in bone tissue regeneration without sintering, to enhance the biofunctionality of scaffolds which retaining mechanical strength. Mechanical stability of the bioceramic scaffold was achieved by adapting a self-setting reaction after material extruding based AM process rather than using a sintering process. Both final crystal state and biodegradability of scaffolds were also controlled by adjusting self-setting reaction. This process could be applied to fabricate various types of bioceramic scaffolds with biofunctional materials, such as osteoblast cells, drugs, biomarkers, and proteins, thereby providing highly functional scaffolds for effective bone tissue regeneration. We believe that this new technology may provide big turning point to overcome limitation of traditional ceramic forming process.

Dr. Hui-Suk Yun

Korea Institute of Materials Science, Korea



Hui-Suk Yun has a Ph. D. on Materials Science Engineering from the University of Tokyo, Japan. She completed her post doc research at National Institute of Advanced Industrial Science and Technology (AIST, Japan) and then worked as a lecturer at the Consolidated Research Institute for Advanced Science and Medical Care at Waseda University, Japan. She is presently working as a principal researcher of Powder and Ceramics Division at Korea Institute of Materials Science (KIMS) and is a professor of Department of Materials Science in University of Science & Technology (UST). She is also working as a R&D Planner of Directorate for National Science and Engineering Programs at National Research Foundation of Korea. Her research field includes the nanoporous materials for both energy- and bio-applications, bioceramics, ceramic additive manufacturing (3D printing) systems & processes, and tissue engineering.

Cluster A

Fundamentals for Materials

Symposium

- A-1** Local Atomic Structure Analysis on the Active Center of Functional Materials
- A-2** Hydrogen in Functional Materials
- A-3** Recent Advances in Computational Materials Science: Bridging Computations and Experiments
- A-4** Neutrons for Materials Research

December 11–12, 2019

Symposium A-1

Local Atomic Structure Analysis on the Active Center of Functional Materials

[Organizers]

Hiroshi DAIMON (Nara Institute of Science and Technology)
 Kouichi HAYASHI (Nagoya Institute of Technology)
 Phil Woodruf (University of Warwick)
 Ian McNulty (MAX IV)

December 11, 2019

Oral Session 1

Time 9:00–11:20 Room Mont-5

Chairperson Hiroshi DAIMON

A1-11-001 ▶ Invited 9:00–9:30

Observing Switching of Ferroelectric Materials by Operando Photoelectron Diffraction

Matthias MUNTWILER¹, Juraj KREMPASKY¹, Hugo DIL^{1,2}

¹Paul Scherrer Institut, ²Ecole Polytechnique Fédérale de Lausanne

A1-11-002 ▶ Invited 9:30–10:00

Holography with Electrons at High Kinetic Energies: Chemical Selective Imaging of Structures at and below Surfaces

Carsten WESTPHAL

TU Dortmund

A1-11-003 10:00–10:20

Atomic image reconstruction from x-ray fluorescence holography and photoelectron holography

Tomohiro MATSUSHITA^{1,2}, Takayuki MURO¹, Naohisa HAPPO³, Koichi HAYASHI²

¹Japan Synchrotron Radiation Research Institute, ²Nara Institute of Science and Technology, ³Hiroshima City University, ⁴Nagoya Institute of Technology

A1-11-004 10:20–10:40

Pressure Driven Superconductivity in Topological Insulators

Yoshihiro KUBOZONO

Research Institute for Interdisciplinary Science, Okayama University

A1-11-005 10:40–11:00

Theory of resonant Auger electron diffraction for active site characterization

Peter KRÜGER¹, Godeung PARK¹, Fumihiko MATSUI²

¹Chiba University, ²Institute for Molecular Science

A1-11-006

11:00–11:20

Analyses of 3D Atomic Arrangements of Dopants in Si Crystal Using Spectro-photoelectron Holography

Kazuo TSUTSUI¹, Kotaro NATORI¹, Tatsuhiko OGAWA¹, Takayuki MURO², Tomohiro MATSUSHITA²,

Yoshitada MORIKAWA³, Takuya HOSHII¹,

Kuniyuki KAKUSHIMA¹, Hitoshi WAKABAYASHI¹,

Kouichi HAYASHI⁴, Fumihiko MATSUI⁵, Toyohiko KINOSHITA²

¹Tokyo Institute of Technology, ²Japan Synchrotron

Radiation Research Institute, ³Osaka University, ⁴Nagoya

Institute of Technology, ⁵Institute of Molecular Science

December 11, 2019

Oral Session 2

Time 14:00–16:00 Room Mont-5

Chairperson Yoshitada MORIKAWA

A1-11-007 ▶ Invited 14:00–14:30

Electronically-driven surface restructuring investigated at the local scale

Karina MORGENSTERN

Ruhr-Universität Bochum

A1-11-008 ▶ Invited 14:30–15:00

How Local Structure Affects CO Binding in Model Ir1/Fe3O4 and Rh1/Fe3O4 Single-Atom Catalysts

Gareth PARKINSON

TU Wien

A1-11-009 15:00–15:20

Concerted Catalysis of Designed Active Sites on Solid Surface for Highly Efficient Organic Synthesis

Ken MOTOKURA¹, Hiroto NODA¹, Yusuke WAKABAYASHI², Hiroo TAJIRI³, Kyogo MAEDA¹, Marika IKEDA¹, Wang-Jae CHUN⁴

¹Tokyo Institute of Technology, ²Tohoku University,

³Japan Synchrotron Radiation Research Institute/SPRING-8,

⁴International Christian University

A1-11-010 15:20–15:40

Determining the dopant site structure in a Rh:SrTiO₃ photocatalyst by x-ray fluorescence holography

Mikk LIPPMAA

University of Tokyo

A1-11-011 15:40–16:00

Middle-range ordering of multi-quantum well (In_{0.1}Ga_{0.9}N/GaN)₂₀ grown on c-face Sapphire Substrate

Tomoaki KAWAMURA¹, Koichi HAYASHI², Munehiko MIYANO¹, Atsushi SAKAKI¹, Akihito ICHIKAWA¹, Jun NAKAMURA³

¹Nichia Corporation, ²Nagoya Institute of Technology,

³The University of Electro-Communications

December 12, 2019

Oral Session 4**Time** 9:00–11:20 **Room** Mont-5

Chairperson Yoshihiro KUBOZONO

A1-12-I01 ▶ Invited 9:00–9:30**The atomic and electronic structure of two-dimensional oxide quasicrystals**

Stefan FÖRSTER¹, Sebastian SCHENK¹, Eva Maria ZOLLNER¹, Cheng-Tien CHIANG¹, Christian TUSCHE^{2,3}, Wolf WIDDRA^{1,2}
¹Martin-Luther-Universität Halle-Wittenberg, ²Max-Planck-Institut für Mikrostrukturphysik, ³Peter-Grünberg-Institut (PGI-6), Forschungszentrum Jülich

A1-12-I02 ▶ Invited 9:30–10:00**Novel 2D Artificial Forms of Elemental Si, Ge, Sn, and Pb : From Silicene to Plumbene**

Guy LE LAY
 Aix-Marseille University

A1-12-003 10:00–10:20**Graphene's Latest Cousin: Plumbene Epitaxial Growth on a "Nano WaterCube"**

Junji YUHARA
 Nagoya University

A1-12-004 10:20–10:40**Nanocrystal Dynamics using Time-resolved Diffracted X-ray Blinking**

YUJI SASAKI^{1,2,3}, M. KURAMOCHI^{1,2}, H. SEKIGUCHI³
¹The University of Tokyo, ²Operand OIL, National Institute of Advanced Industrial Science & Technology, ³Spring-8/Japan Synchrotron Radiation Research Institute

A1-12-005 10:40–11:00**Single-atom Dispersion of Platinum on Graphene using Plasma Sputtering**

Kazutoshi GOHARA, Kenji YAMAZAKI
 Hokkaido University

A1-12-006 11:00–11:20**High-speed X-Ray Reciprocal Space Mapping for Dynamics of Molecular Beam Epitaxy**

Masamitsu TAKAHASHI¹, Wolfgang VOEGELI², Etsuo ARAKAWA², Tetsuro SHIRASAWA³, Takuo SASAKI¹, Tomohiro YAMAGUCHI⁴, Tadashi MATSUSHITA⁵
¹National Institutes for Quantum and Radiological Science and Technology, ²Tokyo Gakugei University, ³National Institute of Advanced Industrial Science and Technology, ⁴Kogakuin University, ⁵High-Energy Accelerator Research Organization

December 12, 2019

Oral Session 5**Time** 14:00–15:50 **Room** Trade-1

Chairperson Tomohiro MATSUSHITA

A1-12-I07 ▶ Invited 14:00–14:30**Large-scale DFT study of complex nano-structured materials with the CONQUEST code**

Tsuyoshi MIYAZAKI
 National Institute for Materials Science (NIMS)

A1-12-008 14:30–14:50**Carrier Transport Calculations of Organic Semiconductors with Static and Dynamic Disorder**

Nobuhiko KOBAYASHI¹, Hiroyuki ISHII¹, Kenji HIROSE²
¹University of Tsukuba, ²NEC

A1-12-009 14:50–15:10**First-principles Theoretical Study on Electronically and Catalytically Active Sites at Graphene**

Yoshitada MORIKAWA^{1,3}, Sasfan Arman WELLA^{1,2}, Fahdzi MUTTAQIEN¹, Suprijadi HARYONO², Kouji INAGAKI^{1,3}, Yuji HAMAMOTO^{1,3}, Ikutaro HAMADA^{1,3}
¹Osaka University, ²Bandung Institute of Technology, ³ESICB, Kyoto University

A1-12-010 15:10–15:30**Statistical and Density-Functional Analysis of the Effect of Heme Porphyrin Distortion in Heme Proteins**

Yu TAKANO^{1,2}, Yusuke KANEMATSU¹, Hiroko X. KONDO^{1,3}, Yasuhiro IMADA²
¹Hiroshima City University, ²Osaka University, ³Kitami Institute of Technology

A1-12-011 15:30–15:50**3D atomic-resolution holography around non-periodic active atoms**

Hiroshi DAIMON
 Toyota Physical and Chemical Research Institute

December 12, 2019

Poster Session**Time** 16:30–18:00 **Room** Trade-0**A1-12-P01****Valence-selective x-ray fluorescence holographic study of YbInCu₄ valence transition material**

Shinya HOSOKAWA¹, Naohisa HAPPO², Kouichi HAYASHI³, Koji KIMURA³, Tomohiro MATSUSHITA⁴, Jens Rüdiger STELLHORN¹, Masaichiro MIZUMAKI⁴, Motohiro SUZUKI⁴, Hitoshi SATO⁵, Koichi HIRAOKA⁶
¹Kumamoto University, ²Hiroshima City University, ³Nagoya Institute of Technology, ⁴JASRI, ⁵Hiroshima University, ⁶Ehime University

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

A1-12-P02

The molecular dynamics simulation on the mechanical properties of Ni glass with external pressure

Liwu JIANG, Peng SHI, Chuanhui ZHANG
University of Science and Technology Beijing

A1-12-P03

Spatiotemporal pattern of graphene ripple structure measured using aberration corrected TEM

Yuhiro SEGAWA, Kenji YAMAZAKI, Kazutoshi GOHARA
Hokkaido University

A1-12-P04

In-situ observation of the motion of single metal atoms on graphene using aberration corrected electron microscopy

Akio SUZUTA, Tsutomu UCHIDA, Kenji YAMAZAKI, Ryo SUGIMOTO, Kazutoshi GOHARA
Hokkaido University

A1-12-P05

K-means clustering based support construction for ptychography

Katsuya ICHIHASHI¹, Shota NOGAWA¹, Yosuke MAEHARA^{1,2}, Hiroyuki SHIOYA¹, Jun YAMASAKI³, Kazutoshi GOHARA⁴
¹Muroran Institute of Technology, ²Dowell Co., Ltd., ³Osaka University, ⁴Hokkaido University

A1-12-P06

Fast Surface X-ray Diffraction for Monitoring of Interface Phenomena

Tetsuro SHIRASAWA
National Institute of Advanced Industrial Science and Technology

A1-12-P07

Evaluation of charge transport property of ethynylene-bridged anthracene oligomers

Juanjuan ZHU, Hironobu HAYASHI, Hiroko YAMADA
Nara Institute of Science and Technology (NAIST)

A1-12-P08

Efficient Hydrosilylation Reaction using Designed Rh Site on Silica Surface

Kyogo MAEDA, Ken MOTOKURA
Tokyo Institute of Technology

A1-12-P09

Fabrication of MoO₃ films on Si(001) by vapor deposition.

Yuya YOSHIE, Shinta KOBAYASHI, Sakura TAKEDA
Nara Institute of Science and Technology

A1-12-P10

Status of photoelectron holography at SPring-8: Experimental setup for time- and space-resolved technique and application to individual atomic imaging of multiple dopant sites

Toyohiko KINOSHITA¹, Tomohiro MATSUSHITA¹, Takayuki MURO¹, Takuo OHKOCHI¹, Hitoshi OSAWA¹, Masaru SHIMOMURA², Fumihiko MATSUI³, Hiroyuki MATSUDA³, Kazuo TSUTSUI⁴, Munetaka TAGUCHI⁵, Kensei TERASHIMA⁶, Takanori WAKITA⁶, Takayoshi YOKOYA⁶, Hiroshi DAIMON⁷
¹Japan Synchrotron Radiation Research Institute (JASRI), ²Department of Engineering, Shizuoka University, ³UVSOR, Institute for Molecular Science, ⁴Institute of Innovative Research, Tokyo Institute of Technology, ⁵Toshiba Nanoanalysis Corporation, ⁶Graduate School of Natural Science and Technology, Okayama University, ⁷Toyota Physical and Chemical Research Institute

A1-12-P11

Self-assembly Material Texture of β -Si₃N₄/Stainless Steel Composites (2)—Effect of Kneading Process and Thermal Conductivity—

Mariko TAKEDA, Kazuya OKUBO, Yuka MIZUKAMI, Yoshihiro SATO, Satoko ABE, Ryota KOBAYASHI, Yue BAO, Fumio MUNAKATA
Tokyo City University

A1-12-P12

Self-assembly Material Texture of β -Si₃N₄/Stainless Steel Composites (3)—Multifractal Analysis of the Aggregated Morphology Texture—

Mariko TAKEDA, Kazuya OKUBO, Yuka MIZUKAMI, Yoshihiro SATO, Satoko ABE, Ryota KOBAYASHI, Yue BAO, Fumio MUNAKATA
Tokyo City University

A1-12-P13

Investigation on Local Crystallographic Structure of ϵ -Ga₂O₃ with High Dielectric Constant

Daichi OKA¹, Subaru YUSA¹, Koji KIMURA², Artoni Kevin Roquero ANG², Naohisa HAPPO³, Kouichi HAYASHI², Tomoteru FUKUMURA^{1,4}

¹Department of Chemistry, Graduate School of Science, Tohoku University, ²Department of Physical Science and Engineering, Nagoya Institute of Technology, ³Department of Computer and Network Engineering, Hiroshima City University, ⁴WPI Advanced Institute for Materials Research and Core Research Cluster, Tohoku University

A1-12-P14

Synthesis and characterization of large acenes by using on-surface synthesis

Hironobu HAYASHI, Hiroko YAMADA
Nara Institute of Science and Technology

A1-12-P15

Analysis of Active Species in Molecular Vanadium Catalysis by Solution XAS Analysis

Kotohiro NOMURA

Tokyo Metropolitan University

A1-12-P16

Improved Phase Imaging by Electron Diffractive Imaging

Jun YAMASAKI^{1,2}, Yuki SHIMAOKA¹, Hirokazu SASAKI³¹Osaka University, ²Nagoya University, ³Furukawa Electric Co., Ltd

A1-12-P17

Benchmark Study on Bond Dissociation Energies for Large Systems

Toru SAITO, Hiroki KAMBARA, Seiya YAMAMOTO, Yu TAKANO

Hiroshima City University

A1-12-P18

Dehydrogenative Arene Coupling of Dimethyl Phthalate: The Role of Pd and Cu Catalysts

Masafumi HIRANO¹, Yuki KANAZAWA¹, Takato MITSUDOME², Kousuke SANŌ¹¹Tokyo University of A & T, ²Osaka University

A1-12-P19

Band Alignment of Lattice-Matched ZnSnAs₂/InP HeterostructuresMunetaka TAGUCHI¹, Naomi KURIHARA¹, Teruhiko SAZE¹, Kei KIYOKAWA¹, Hitoshi SATO³, Naotaka UCHITOMI², Hiroto OOMAE²¹Toshiba Nanoanalysis Corporation, ²Nagaoka University of Technology, ³Hiroshima University

A1-12-P20

Formic Acid Adsorption and Decomposition on the Cu(111) Surface: Monomeric and Polymeric Structures Study

Septia Eka Marsha PUTRA¹, Fahdzi MUTTAQIEN¹, Yuji HAMAMOTO^{1,2}, Kouji INAGAKI^{1,2}, Ikutaro HAMADA^{1,2}, Yoshitada MORIKAWA^{1,2,3}¹Department of Precision Science and Technology, Graduate School of Engineering, Osaka University, ²Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, ³Research Center for Ultra-Precision Science and Technology, Graduate School of Engineering, Osaka University

A1-12-P21

Pressure Dependence of Superconductivity in SrIr₂ and BaIr₂

Huan LI

Okayama University

A1-12-P22

Revealing the effect of Co loading on the morphology and activity of Co/Co_{1-x}Al_{2+x}O₄ catalysts for dry reforming of methaneYee Jie WONG^{1,2}, Mei Kee KOH², Satoshi ICHIKAWA¹, Yoshitada MORIKAWA¹, Abdul Rahman MOHAMED²¹Osaka University, ²Universiti Sains Malaysia

A1-12-P23

Preparation and Characterization of Superconducting Ba_{1-x}M_xTi₂Sb₂O (M: Na, K, Rb and Cs)

Yanan WANG

Okayama University

A1-12-P24

Structural Isomerization of Phosphine-Protected Metal Clusters Induced by Polyoxometalates

Yu FUJIKI¹, Tomoki MATSUYAMA¹, Hikaru TAKAYA², Nobuhiro YASUDA³, Naoki NAKATANI¹, Jun HIRAYAMA⁴, Seiji YAMAZOE^{1,4,5}¹School of Science, Tokyo Metropolitan University, ²Institute for Chemical Research, Kyoto University, ³Japan Synchrotron Radiation Research Institute, ⁴Elements Strategy Initiative for Catalysts and Batteries, Kyoto University, ⁵Core Research for Evolutional Science and Technology, Japan Science and Technology Agency

A1-12-P25

First principles study for electronic structure of Nitrogen-doped TiO₂(B)Tomoki YUYAMA¹, Carla BITTENCOURT², Peter KRÜGER¹¹Chiba University, ²University of Mons

A1-12-P26

Comparative and Systematic Study of Doping Technology for 2D-Sputtered MoS₂ Film

Takuya HAMADA, Shimpei YAMAGUCHI, Taiga HORIGUCHI, Kuniyuki KAKUSHIMA, Kazuo TSUTSUI, Hitoshi WAKABAYASHI

Tokyo Institute of Technology

A1-12-P27

X-ray Fluorescence Holographic Imaging of Iron Environments in Heme Proteins

Ayana SATO-TOMITA

Jichi Medical University

A1-12-P28

QM/MM study of the ATPase mechanism of F-actin

Yusuke KANEMATSU¹, Yu TAKANO¹, Shuichi TAKEDA², Ryotaro KOIKE², Motonori OTA², Yuichiro MAEDA²¹Hiroshima City University, ²Nagoya University

A1-12-P29

Self-assembly Material Texture of β -Si₃N₄ /Stainless Steel Composites (1)—Effect of Firing Process on the Formation of Agglomerated Texture—

Masashi KOGA, Mariko TAKEDA, Kazuya OKUBO, Yuka MIZUKAMI, Yoshihiro SATO, Satoko ABE, Ryota KOBAYASHI, Yue BAO, Fumio MUNAKATA
Tokyo City University

A1-12-P30

Study of graphene precipitation from Ni catalyst using in-situ X-ray diffraction measurement - Cooling rate dependence -

Jumpei YAMADA, Yuki UEDA, Daichi YAMAMOTO, Takahiro MARUYAMA, Shigeya NARITSUKA
Meijo University

A1-12-P31

Local Dynamics of bio-soft materials using synchrotron radiation X-ray and nanocrystals

Hiroshi SEKIGUCHI¹, Yuji C. SASAKI²
¹Japan Synchrotron Radiation Research Institute, ²The University of Tokyo

A1-12-P32

Modification of graphite energy analyzer for light elements on X-ray fluorescence holography

Naohisa HAPPO¹, Atsushi KUBOTA¹, Tomohiro MATSUSHITA², Shinya HOSOKAWA³, Koji KIMURA⁴, Kouichi HAYASHI⁴
¹Hiroshima City University, ²Japan Synchrotron Radiation Research Institute, ³Kumamoto University, ⁴Nagoya Institute of Technology

A1-12-P33

Observation of doping effect in Sm doped RB₆ (R: rare earth) by white neutron holography

Shoichi UECHI¹, Yuki KANAZAWA¹, Kazuya SUGIMOTO¹, Takayoshi YAMAMOTO¹, Kenji OHYAMA¹, Naohisa HAPPO², Kouichi HAYASHI³, Masahide HARADA⁴, Kenichi OIKAWA⁴, Yasuhiro INAMURA⁴, Wataru MATSUHARA¹, Fumitoshi IGA¹, Youhei FUKUMOTO¹
¹Ibaraki University, ²Hiroshima City University, ³Nagoya Institute of Technology, ⁴J-PARC Center

A1-12-P34

Determination of dopant position of thermoelectric material B-doped Mg₂Si by white neutron holography

Kazuya SUGIMOTO¹, Syouichi UECHI¹, Yuki KANAZAWA¹, Yohei FUKUMOTO¹, Takayoshi YAMAMOTO¹, Kenji OHYAMA¹, Kouichi HAYASHI², Naohisa HAPPO³, Masahide HARADA⁴, Kenichi OIKAWA⁴, Yasuhiro INAMURA⁴, Kei HAYASHI⁵, Wataru SAITOU⁵, Yuzuru MIYAZAKI⁵
¹Ibaraki University, ²Nagoya Institute of Technology, ³Hiroshima City University, ⁴Materials and Life Science Division, J-PARC Center, ⁵Tohoku University

A1-12-P35

Valence sensitive X-ray fluorescence holography of the protein complex Photosystem II

Koichi HAYASHI¹, Artoni Kevin Roquero ANG¹, Yasushi UMENA², Ayana SATO-TOMITA³, Naoya SHIBAYAMA³, Yuji SASAKI⁴, Naohisa HAPPO⁵, Koji KIMURA¹
¹Nagoya Institute of Technology, ²Okayama University, ³Jichi Medical University, ⁴The University of Tokyo, ⁵Hiroshima City University

A1-12-P36

Atomic and electronic structure analysis of metallic nanoparticle catalysts by large-scale DFT calculations

Ayako NAKATA, Tsuyoshi MIYAZAKI
National Institute for Materials Science

A1-12-P37

Active/Inactive Dopant-site in Boron-doped Diamond in Diamond Power Device

Yukako KATO
National Institute of Advanced Industrial Science and Technology

A1-12-P38

Structural Evolution During Photo- and Thermal Conversion of Organic Semiconductor Precursor Thin Films

Wolfgang VOEGELI¹, Yuta TAMEIKE¹, Atsushi YAMAGUCHI¹, Ryoma TANAKA¹, Etsuo ARAKAWA¹, Toshio TAKAHASHI¹, Tetsuroh SHIRASAWA², Mitsuharu SUZUKI³, Hiroko YAMADA⁴
¹Tokyo Gakugei Univ., ²AIST, ³Osaka Univ., ⁴NAIST

A1-12-P39

Convergent-Beam Optics for Time-Resolved X-Ray Diffraction From Thin Films and Surfaces

Wolfgang VOEGELI¹, Masamitsu TAKAHASHI², Takuo SASAKI², Seiji FUJIKAWA², Tetsuroh SHIRASAWA³, Etsuo ARAKAWA¹, Tadashi MATSUSHITA⁴
¹Tokyo Gakugei Univ., ²QST, ³AIST, ⁴KEK

A1-12-P40

A Plan of Photoelectron Holography at MAX IV

Yusuke HASHIMOTO^{1,2}, Balasubramanian THIAGARAJAN², Conny SÄTHE², Oscar TJERNBERG¹
¹KTH Royal Institute of Technology, ²Max IV Laboratory

A1-12-P41

Acceleration of Atomic Image Reconstruction from X-ray Fluorescence Holograms on Multiple Platforms

Atsushi KUBOTA¹, Tomohiro HARA¹, Tomohiro MATSUSHITA², Naohisa HAPPO¹, Tetsuo HIRONAKA¹
¹Hiroshima City University, ²Japan Synchrotron Radiation Research Institute

A1-12-P42

Local Atomic Arrangement near Co and Ni in an Aged $Al_{0.3}CrFeCoNi$ High Entropy Alloy

Jumpei NIKI¹, Tatsuya HAYASHI¹, Tokujiro YAMAMOTO¹, Naohisa HAPPO², Kouichi HAYASHI³, Koji KIMURA³, Shinya HOSOKAWA⁴, Hiroo TAJIRI⁵

¹Utsunomiya University, ²Hiroshima City University, ³Nagoya Institute of Technology, ⁴Kumamoto University, ⁵Japan Synchrotron Radiation Research Institute

A1-12-P43

Time Dependence of Vickers Hardness and X-ray Fluorescence Holograms of an $Al_{0.3}CrFeCoNi$ High Entropy Alloy

Tokujiro YAMAMOTO¹, Jumpei NIKI¹, Tatsuya HAYASHI¹, Naohisa HAPPO², Kouichi HAYASHI³, Koji KIMURA³, Shinya HOSOKAWA⁴, Hiroo TAJIRI⁵

¹Utsunomiya University, ²Hiroshima City University, ³Nagoya Institute of Technology, ⁴Kumamoto University, ⁵Japan Synchrotron Radiation Research Institute

A1-12-P44

A Middle Energy-bandwidth Crystal Monochromator using Asymmetric Geometry for High-flux Synchrotron X-ray Diffraction

Hiroo TAJIRI¹, Hiroshi YAMAZAKI¹, Haruhiko OHASHI¹, Shunji GOTO¹, Osami SAKATA², Tetsuya ISHIKAWA³

¹Japan Synchrotron Radiation Research Institute, ²National Institute for Materials Science, ³RIKEN SPring-8 Center

A1-12-P45

Development of High-Energy-Resolution Display-type Analyzer

Hiroshi DAIMON¹, Hiroyuki MATSUDA¹, Hiroki MOMONO¹, László TÓTH²

¹Nara Institute of Science and Technology (NAIST), ²University of Debrecen, ³Toyota Physical and Chemical Research Institute

A1-12-P46

X-ray Fluorescence Holography Investigation on Sn in Sn: β -Ga₂O₃ widegap oxide semiconductor

Kazushi MIKI¹, N HAPPO², K KIMURA³, K SASAKI⁴, Y TANG¹, K NAWATA¹, Y MAEDA¹, S KITAMURA¹, H OZAKI³, H HISATUNE², R YAMAGUCHI², H TAJIRI⁵, S YAMAKOSHI⁶, A KURAMATA⁴

¹Univ. Hyogo, ²Hiroshima City Univ., ³Nagoya Institute of Technology, ⁴Novel Crystal Technology, Inc., ⁵JASRI, ⁶Tamura Corp.

A1-12-P47

Experimental Investigation of the Local Atomic Structure in Decagonal Quasicrystals by X-Ray Fluorescence Holography

Jens STELLHORN
DESY

A1-12-P48

Molecular dynamics study of structural fluctuations in CDR-H3 of anti-HIV antibodies PG9 and PG16

NAOKI TANABE¹, RYO KIRIBAYASI¹, Hiroko.X KONDO², DAISUKE KURODA³, TORU SAITO¹, JIRO KOHDA¹, AKIMITSU KUGIMIYA¹, YASUHISA NAKANO¹, KOUHEI TSUMOTO^{3,4}, YU TAKANO¹

¹Graduate School of Information Sciences, Hiroshima City University, ²Faculty of Engineering, Kitami Institute of Technology, ³Institute of Medical science, the University of Tokyo, ⁴Graduate School of Engineering, the University of Tokyo

December 12–13, 2019

Symposium A-2

Hydrogen in Functional Materials

[Organizers]

Shin-ichi ORIMO (Tohoku University, Japan)
 Hidenori HIRAMATSU (Tokyo Institute of Technology, Japan)
 Bjørn C. HAUBACK (Institute for Energy Technology, Norway)
 Truls NORBY (University of Oslo, Norway)
 Chris G. Van de WALLE (University of California, Santa Barbara, USA)

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December 12, 2019

Oral Session 4

Time 9:30–12:15 Room Ken-2

Chairpersons Hiroshi KAGEYAMA, Tom AUTREY

A2-12-K01 ▶ Keynote 9:30–10:15

Enabling Energy Technologies Using Hydride Materials

Rana MOHTADI

TOYOTA RESEARCH INSTITUTE OF NORTH AMERICA

A2-12-I02 ▶ Invited 10:15–10:45

Complex Hydrides for Energy Device Research

Shin-ichi ORIMO

Tohoku University

A2-12-003 10:45–11:05

Molecular Dynamics Study of Fast Li⁺ Ion Transport in *closo*-Boranes.

Kartik SAU¹, Tamio IKESHOJI^{1,2}, Shigeyuki TAKAGI³,
 Kazuto AKAGI³, SHIN-ICHI ORIMO^{2,3}, Sangryun KIM³

¹AIST-TohokuU Mathematics for Advanced Materials-OIL,

²IMR, Tohoku University, ³AIMR, Tohoku University

Break

11:05–11:15

A2-12-I04 ▶ Invited 11:15–11:45

Hydride ion conduction

Truls NORBY, Xin LIU, Tor S. BJØRHEIM, Reidar HAUGSRUD

University of Oslo

A2-12-I05 ▶ Invited 11:45–12:15

Size Flexibility of Hydride Anion: Structure and Property Control

Hiroshi KAGEYAMA

Kyoto University

December 12, 2019

Oral Session 5

Time 14:00–16:30 Room Ken-2

Chairpersons Anderson JANOTTI, Truls NORBY

A2-12-006 14:00–14:20

H⁻ Conduction in the Rock-Salt Layer of K₂NiF₄-Type Oxyhydrides

Genki KOBAYASHI^{1,2}, Fumitaka TAKEIRI^{1,2},
 Akihiro WATANABE^{1,3}, Haq NAWAZ^{1,2}, Akihide KUWABARA⁴,
 Yumiko IMAI¹, Nur Ika Puji AYU^{1,5}, Masao YONEMURA⁵,
 Ryoji KANNO³

¹Institute for Molecular Science, ²SOKENDAI, ³Tokyo
 Institute of Technology, ⁴Japan Fine Ceramics Center,

⁵High Energy Accelerator Research Organization

A2-12-007 14:20–14:40

Characteristic H⁻ Ion Conduction in Oxygen-Substituted Lanthanum Trihydride

Soshi IIMURA¹, Keiga FUKUI¹, Tomofumi TADA¹,
Satoru FUJITSU¹, Masato SASASE¹, Hiromu TAMATSUKURI²,
Takashi HONDA², Kazutaka IKEDA², Toshiya OTOMO²,
Hideo HOSONO¹

¹Tokyo Institute of Technology, ²High Energy Accelerator
Research Organization (KEK)

A2-12-008 14:40–15:00

Fast Hydride Ionic Conduction of Lanthanum Oxyhydride from First Principles Molecular Dynamics Simulation

Tomofumi TADA, Soshi IIMURA, Hideo HOSONO
Tokyo Institute of Technology

Break
15:00–15:10

A2-12-109 ▶ Invited 15:10–15:40

Catalytic Properties of Hydrides in Aqueous Media

Tom AUTREY
Pacific Northwest National Laboratory

A2-12-110 ▶ Invited 15:40–16:10

Inorganic Nanomaterials to Achieve Efficient Electrochemical Hydrogenation for Energy Storage and Materials Conversions

Miho YAMAUCHI
Kyushu University

A2-12-011 16:10–16:30

Hydrogen storage behaviors and application for ammonia synthesis of LnNiSi (Ln = La–Nd)

Hiroshi MIZOGUCHI¹, Sang-Won PARK¹, Kazuhisa KISHIDA¹,
Masaaki KITANO¹, Junghwan KIM¹, Masato SASASE¹,
Takashi HONDA², Kazutaka IKEDA², Toshiya OTOMO²,
Hideo HOSONO¹

¹Tokyo Institute of Technology, ²KEK

December 13, 2019

Oral Session 7

Time 9:30–11:45 **Room** Ken-2

Chairperson Miho YAMAUCHI

A2-13-K01 ▶ Keynote 9:30–10:15

Investigation on Defect Structures in Oxides with Hydrogen Impurity

Naoki OHASHI^{1,2,3}
¹National Institute for Materials Science, ²Tokyo Institute of
Technology, ³Kyushu University

A2-13-102 ▶ Invited 10:15–10:45

The hydrogen impurity in wide-band-gap oxides

Anderson JANOTTI
University of Delaware

A2-13-003 10:45–11:05

Structures and Electronic States of Hydrogen in Inorganic Semiconductors with Different Anions

Toshio KAMIYA, Xinyi HE, Zewen XIAO, Keisuke IDE,
Takayoshi KATASE, Hideo HOSONO
Tokyo Institute of Technology

A2-13-004 11:05–11:25

Hydrogen Doping in Ultra-widegap Amorphous Oxide Semiconductor, Amorphous Ga-O

Keisuke IDE^{1,2}, Yurika KASAI¹, Takayoshi KATASE^{1,3},
Hidenori HIRAMATSU^{1,2}, Hideo HOSONO^{1,2}, Toshio KAMIYA^{1,2}
¹Laboratory for Materials and Structures, Tokyo Institute
of Technology, ²Materials Research Center for Element
Strategy, Tokyo Institute of Technology, ³PRESTO, Japan
Science and Technology Agency

A2-13-005 11:25–11:45

Activation energy of hydrogen effusion of high performance TiO_x/SiO_x/c-Si heterocontacts

Kazuhiro GOTOH¹, Takeya MOCHIZUKI¹, Tomohiko HOJO²,
Yasuyoshi KUROKAWA¹, Eiji AKIYAMA², Noritaka USAMI¹
¹Nagoya University, ²Tohoku University

December 13, 2019

Oral Session 8

Time 14:00–15:40 **Room** Ken-2

Chairperson Genki KOBAYASHI

A2-13-006 14:00–14:20

Kinetic Enhancement of Hydrogen Absorption by Pd through Surface Modification with Au

Shohei OGURA, Kazuhiro NAMBA, Koichi KATO,
Katsuyuki FUKUTANI
Institute of Industrial Science, The University of Tokyo

A2-13-007 14:20–14:40

Caught in the Act: Hydrogen Bond at Work in Asymmetric Synthesis Monitored by Modulation-Excitation Infrared Spectroscopy

Nobutaka MAEDA, Miho YAMAUCHI
Kyushu University, International Institute for Carbon-
Neutral Energy Research (WPI-I2CNER)

A2-13-008 14:40–15:00

Hydride Complexes with High Hydrogen Coordination and Their Novel Functionalities

Shigeyuki TAKAGI¹, Shin-ichi ORIMO^{1,2}
¹Institute for Materials Research, Tohoku University / Japan,
²WPI-Advanced Institute for Materials Research (AIMR),
Tohoku University / Japan

A2-13-009

15:00–15:20

High-pressure and high-temperature synthesis of novel hydrides

 Hiroyuki SAITOH^{1,2}, Mai TANIKAMI^{1,2}, Akihiko MACHIDA¹, Tetsu WATANUKI^{1,2}, Toyoto SATO³, Shigeyuki TAKAGI³, Shin-ichi ORIMO^{3,4}, Kazutaka IKEDA⁴, Toshiya OTOMO⁴
¹National Institutes for Quantum and Radiological Science and Technology, ²Graduate School of Material Science, Univ. of Hyogo, ³Institute for Materials Research, Tohoku University, ⁴WPI-Advanced Institute for Materials Research (AIMR), Tohoku University, ⁵Institute of Materials Structure Science, High Energy Accelerator Research Organization

A2-13-010

15:20–15:40

Magnetic structure of heavily hydrogen-substituted 1111-type LaMnPO_{1-x}H_x

 Satoru MATSUISHI¹, Toshiki KATO¹, Tomohiro INOUE¹, Maxim AVDEEV², Yusuke NAMBU³
¹Materials Research Center for Element Strategy, Tokyo Institute of Technology, ²Bragg Institute, Australian Nuclear Science and Technology Organization, ³Institute for Materials Research, Tohoku University

December 13, 2019

Oral Session 9

Time 16:30–17:30 Room Ken-2

Chairperson Hiroyuki SAITOH

A2-13-011

16:30–16:50

First-principles calculations of hydrogen-related reactions in polymer electrolyte fuel cell

Yoshiyuki YAMAMOTO, Lei YAN, Osamu SUGINO

The Institute for Solid State Physics, The University of Tokyo

A2-13-012

16:50–17:10

Proton conduction on hydrated oxide surface for “electrolyte” of metal/oxide catalysts

 Ryuhei SATO¹, Yasushi SHIBUTA¹, Fuyuki SHIMOJO², Shu YAMAGUCHI³
¹The University of Tokyo, ²Kumamoto University, ³National Institution for Academic Degrees and Quality Enhancement of Higher Education

A2-13-013

17:10–17:30

Sulfonated Poly(arylene perfluoroalkylene) Terpolymers as Proton Exchange Membranes

Zhi LONG, Junpei MIYAKE, Kenji MIYATAKE

University of Yamanashi

December 13, 2019

Poster Session

Time 19:00–20:30 Room Trade-0

A2-13-P01

Development of highly hydrogen-sensitive thermal desorption spectroscopy system for quantitative analysis of low hydrogen concentration ($\sim 1 \times 10^{16}$ atoms/cm³) in thin-film samples

 Hidenori HIRAMATSU¹, Taku HANNA¹, Isao SAKAGUCHI², Hideo HOSONO¹
¹Tokyo Institute of Technology, ²National Institute for Materials Science

A2-13-P02

Effective interaction for vanadium oxyhydrides
Sr_{n+1}V_nO_{2n+1}H_n (n = 1 and ∞): A constrained-RPA study

Masayuki OCHI, Kazuhiko KUROKI

Osaka University

A2-13-P03

Hydride ion in iron-based superconductors: Efficient electron dopant inducing high-T_c superconductivity and antiferromagnetism

Soshi IIMURA, Hideo HOSONO

Tokyo Institute of Technology

A2-13-P04

Crystal Structures and Photochromic Reactions of Hydrogen-Bonding Diarylethene Crystals

Masakazu MORIMOTO

Rikkyo University

A2-13-P05

Theoretical Study of Hydrogen/Deuterium Absorption Properties in Pd By Using Combined Plane Wave and Localized Basis Set Approach

Takayoshi ISHIMOTO

Yokohama City University

A2-13-P06

Research on Ammine Complex of Metal Borohydrides as Functional Material

Hiroki MIYAOKA, Keita NAKAJIMA, Takayuki ICHIKAWA,

Yoshitsugu KOJIMA

Hiroshima University

A2-13-P07

Investigation of cathodic reaction of proton-conducting ceramics fuel cells by using model pattern electrodes

 Takashi NAKAMURA¹, Katsuya NISHIDATE², Yuta KIMURA¹, Keiji YASHIRO³, Tatsuya KAWADA³, Yuichi MIKAMI⁴, Tomohiro KUROHA⁴, Yoichiro TSUJI⁴, Koji AMEZAWA¹
¹IMRAM, Tohoku University, ²Dept. Mech. Sys. Eng., Grad. School of Engineering, Tohoku University, ³Grad. School of Environmental Studies, Tohoku University, ⁴Panasonic Corp.

A2-13-P08

Theoretical study of H/D isotope effect on phase transition of hydrogen-bonded organic conductor $\kappa\text{-H}_3(\text{Cat-EDT-TTF})_2$

Masanori TACHIKAWA
Yokohama City University

A2-13-P09

Control of electrical properties on transition metal oxides via protonic-electronic coupling

Hidekazu TANAKA, Azusa. N. HATTORI, Takashi YAMANAKA, Daiki KAWAMOTO, Keiichiro HAYASHI
Osaka University

A2-13-P10

Local electronic structure of interstitial hydrogen in manganese dioxide

Hirotaoka OKABE¹, Ryosuke KADONO¹, Masatoshi HIRAISHI¹, Akihiro KODA¹, Soshi TAKESHITA¹, Kenji KOJIMA², Ichihiko YAMAUCHI³, Hirohiko SATO⁴
¹High Energy Accelerator Research Organization (KEK), ²TRIUMF, ³Saga University, ⁴Chuo University

A2-13-P11

Moved

A2-13-P12

Lanthanide Oxyhydrides supported Ruthenium catalysts for ammonia synthesis

Masaaki KITANO¹, Kayato Ooya¹, Keiga FUKUI¹, Soshi IIMURA¹, Tomofumi TADA¹, Hideo HOSONO¹
¹Tokyo Institute of Technology, ²Precursory Research for Embryonic Science and Technology

A2-13-P13

Heavy Hydrogen-doping of an Iron-based Superconductor SmFeAsO Epitaxial Film

Jumpei MATSUMOTO¹, Kota HANZAWA¹, Masato SASASE², Silvia HAINDL³, Takayoshi KATASE¹, Hidenori HIRAMATSU^{1,2}, Hideo HOSONO^{1,2}
¹Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology, ²Materials Research Center for Element Strategy, Tokyo Institute of Technology, ³World Research Hub Initiative (WRHI), Institute of Innovative Research, Tokyo Institute of Technology

A2-13-P14

Carbon Doping of Hydrogen Boride Sheet Reduces H_2 Release Temperature

Takahiro KONDO^{1,2}, Yoshitaka FUJIMOTO³, Ryota ISHIBIKI⁴, Taiga GOTO⁴, Shin-ichi ITO^{1,2}, Takeshi FUJITA⁵, Akiyasu YAMAMOTO^{2,6}, Susumu SAITO^{2,3}, Hideo HOSONO²
¹Faculty of Pure and Applied Sciences, University of Tsukuba, ²Materials Research Center for Element Strategy, Tokyo Institute of Technology, ³Department of Physics, Tokyo Institute of Technology, ⁴Graduate School of Pure and Applied Sciences, University of Tsukuba, ⁵School of Environmental Science and Engineering, Kochi University of Technology, ⁶Institute of Engineering, Tokyo University of Agriculture and Technology

A2-13-P15

Hydrogenated Borophene Shows Catalytic Activity as Solid Acid

Takahiro KONDO^{1,3}, Asahi FUJINO², Shin-ichi ITO^{1,3}, Taiga GOTO², Ryota ISHIBIKI², Junko N KONDO⁴, Tadahiro FUJITANI^{1,5}, Junji NAKAMURA¹, Hideo HOSONO³
¹Faculty of Pure and Applied Sciences, University of Tsukuba, ²Graduate School of Pure and Applied Sciences, University of Tsukuba, ³Materials Research Center for Element Strategy, Tokyo Institute of Technology, ⁴IIR, Tokyo Institute of Technology, ⁵Interdisciplinary Research Center, AIST

A2-13-P16

Fast H^- conduction in lanthanum oxyhydride $\text{LaH}_{3-2x}\text{O}_x$

Keiga FUKUI¹, Soshi IIMURA¹, Tomofumi TADA¹, Satoru FUJITSU³, Masato SASASE¹, Hiromu TAMATSUKURI², Takashi HONDA², Kazutaka IKEDA², Toshiya OTOMO², Hideo HOSONO¹
¹MCES, Tokyo Institute of Technology, ²High Energy Accelerator Research Organization (KEK)

A2-13-P17

The role of anion order/disorder in the hydride conductivity in LnHO

Hiroki UBUKATA¹, Thibault BROUX¹, Fumitaka TAKEIRI^{2,3}, Kazuki SHITARA³, Hiroki YAMASHITA¹, Akihito KUWABARA⁵, Genki KOBAYASHI^{2,3}, Hiroshi KAGEYAMA¹
¹Kyoto University, ²Institute for Molecular Science, ³SOKENDAI (The Graduate University for Advanced Studies), ⁴Osaka University, ⁵Japan Fine Ceramics Center

A2-13-P18

Effect of cation size on hydride ion conduction in $\text{LnSrLiH}_2\text{O}_2$ ($\text{Ln} = \text{La, Pr, Nd, Sm, Gd}$) oxyhydrides

Naoki MATSUI¹, Yoyo HINUMA^{2,3}, Yuki IWASAKI¹, Kota SUZUKI¹, Jiang GUANGZHONG¹, Haq NAWAZ^{4,5}, Yumiko IMAI⁴, Masao YONEMURA⁶, Masaaki HIRAYAMA¹, Genki KOBAYASHI^{4,5}, Ryoji KANNO¹
¹Tokyo Institute of Technology, ²Chiba University, ³National Institute for Materials Science, ⁴Institute for Molecular Science, ⁵SOKENDAI (The Graduate University for Advanced Studies), ⁶High Energy Accelerator Research Organization (KEK)

A2-13-P19

Hydrogen Anion and Subgap States in Amorphous In-Ga-Zn-O Thin Films

Joonho BANG, Satoru MATSUSHI, Hideo HOSONO
Tokyo Institute of Technology

A2-13-P20

Synthesis, local electronic structure and photoluminescence properties of rare earth-activated aluminate oxyhydride $\text{Sr}_3\text{AlO}_4\text{H}$.

Tong WU, Satoru MATSUSHI
Tokyo Institute of Technology

A2-13-P21
Adsorption of CO₂ on Hydrogen Boride Sheets with H-vacancy Defects

Taiga GOTO¹, Ryota ISHIBIKI¹, Shin-ichi ITO^{2,3},
Hideo HOSONO², Takahiro KONDO³

¹Graduate School of Pure and Applied Sciences, University of Tsukuba, ²Materials Research Center for Element Strategy, Tokyo Institute of Technology, ³Faculty of Pure and Applied Sciences, University of Tsukuba

A2-13-P22
Structure and Electronic States Changes of Hydrogen Boride Sheets with Heating

Ryota ISHIBIKI¹, Iwao MATSUDA², Shin-ichi ITO^{3,4},
Hideo HOSONO³, Takahiro KONDO^{3,4}

¹Graduate school of Pure and Applied Sciences, University of Tsukuba, ²Institute for Solid State Physics, University of Tokyo, ³Materials Research Center for Element Strategy, Tokyo Institute of Technology, ⁴Faculty of Pure and Applied Sciences, University of Tsukuba

A2-13-P23
Epitaxial growth of Ca₂NH thin films using reactive magnetron sputtering.

Seoungmin CHON¹, Shigeru KOBAYASHI¹, Kazunori NISHIO¹,
Ryota SHIMIZU^{1,2}, Taro HITOSUGI¹

¹Tokyo Institute of Technology, ²JST-PRESTO

A2-13-P24
Molecular Dynamics and Kinetic Monte Carlo Hybrid Method for Efficient Dynamics and Proton Conduction in Phosphoric Acid

Albert ISKANDAROV, Tomofumi TADA

Materials Research Center for Element Strategy, Tokyo Institute of Technology

A2-13-P25
Light-induced Large Electrical Resistivity Reduction in Yttrium Oxy-hydride Epitaxial Thin Films

Yuya KOMATSU¹, Ryota SHIMIZU^{1,2}, Kazunori NISHIO¹,
Masahiro MIYAUCHI¹, Markus WILDE³,
Katsuyuki FUKUTANI³, Taro HITOSUGI¹

¹Tokyo Institute of Technology, ²JST-PRESTO, ³Univ. of Tokyo

A2-13-P26
Passivation of Deep centers in Zinc Oxide Studied with Deep Level Transient Spectroscopy

Takeo OHSAWA

National Institute for Materials Science

A2-13-P27
Photo-induced color centers creation in Sr₂LiSiO₄H oxyhydride

Fauzin NAIMAH, Tong WU, Asako ISHIKAWA,
Satoru MATSUISHI

Tokyo Institute of Technology

A2-13-P28
Low temperature synthesis of perovskite-type oxynitride-hydride as a catalyst for ammonia synthesis

Jun KUJIRAI, Masaaki KITANO, Kiya OGASAWARA,
Tomofumi TADA, Hideo HOSONO

Tokyo Institute of Technology

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 11, 2019

Symposium A-3**Recent Advances in Computational Materials Science: Bridging Computations and Experiments**

[Organizers]

Taisuke OZAKI

(Institute for Solid State Physics, The University of Tokyo)

Minoru OTANI

(National Institute of Advanced Industrial Science and Technology)

December 11, 2019

Oral Session 1

Time 9:00–11:35 Room Mont-2

Chairperson Taisuke OZAKI

A3-11-001 ▶ Invited 9:00–9:40

Construction and exploitation of large ab initio data spaces to design materials with superior mechanical propertiesJoerg NEUGEBAUER

Max-Planck-Institut fuer Eisenforschung

A3-11-002 9:40–10:05

A Prototype First-Principles Only Phase Diagram: Al-NiTheresa DAVEY, Nguyen-Dung TRAN,
Arkapol SAENGDEEJING, Ying CHEN

School of Engineering, Tohoku University

A3-11-003 10:05–10:30

Python Framework for Direct Coupling of First-Principles Calculation with Replica Exchange Monte Carlo Sampling of Ion Disorder in SolidsShusuke KASAMATSU^{1,2}, Yuichi MOTOYAMA²,
Yoshiyuki YAMAMOTO², Kazuyoshi YOSHIMI²,
Taisuke OZAKI², Osamu SUGINO²¹Yamagata University, ²University of Tokyo[Break
10:30–10:45]

A3-11-004 10:45–11:10

First-principles prediction of structural phase transition temperature of BaTiO₃ based on finite-temperature phonon calculationDaisuke HIRAI¹, Sakyo HIROSE¹, Terumasa TADANO²¹Murata Manufacturing Co., Ltd., ²National Institute for Materials Science

A3-11-005

11:10–11:35

Lattice thermal conductivity simulations by high-dimensional neural network potentialsEmi MINAMITANI¹, Masayoshi OGURA²,
Satoshi WATANABE^{2,3}¹Institute for Molecular Science, ²Department of Materials Engineering, the University of Tokyo, ³Center for Materials Research by Information Integration, Research and Services Division of Materials Data and Integrated System, National Institute for Materials Science

December 11, 2019

Oral Session 2

Time 14:00–15:55 Room Mont-2

Chairperson Minoru OTANI

A3-11-006 14:00–14:25

Insulator-Metal transition by non-adiabatic quantum lattice fluctuationsNorikazu TOMITA¹, Akira TAKAHASHI²¹Yamagata University, ²Nagoya Institute of Technology

A3-11-007 14:25–14:50

Structure map for AB₂ type 2D monolayers by high-throughput DFT calculationsMasahiro FUKUDA¹, Jingning ZHANG², Yung-Ting LEE¹,
Taisuke OZAKI¹¹University of Tokyo, ²University of Science and Technology of China[Break
14:50–15:05]

A3-11-008 15:05–15:30

Niobium oxide dihalides NbOX₂: a new family of two-dimensional van der Waals layered materials with intrinsic ferroelectricity and antiferroelectricityGaoyang GOU

Xi'an Jiaotong University

A3-11-009 15:30–15:55

Small Polarons in BaTiO₃: A First-Principles StudyNaoki TSUNODA¹, Yu KUMAGAI², Fumiyasu OBA^{1,2}¹Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology, ²Materials Research Center for Element Strategy, Tokyo Institute of Technology

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 11, 2019

Poster Session

Time 19:00–20:30 Room Trade-0

A3-11-P01
High-throughput Force Field Calculation towards the Search for Fast Ion Conductive Materials

 Yasuhiro MIYAJI¹, Kouki NAKANO¹, Naoto TANIBATA^{1,2}, Ryo KOBAYASHI^{1,3}, Masanobu NAKAYAMA^{1,2,3}
¹Nagoya Institute of Technology, ²Kyoto University ESICB of Elements Strategy Initiative for Catalysts and Batteries, ³MaDis/CMi2, NIMS of National Institute for Materials Science

A3-11-P02
Theoretical Study of Singlet Exciton Fission in Organic Materials

Hiroyuki TAMURA

The University of Tokyo

A3-11-P03
Temperature Dependent Grain Boundary Segregation in BCC-Fe – A Grand Canonical Monte Carlo – Molecular Dynamics Hybrid Study

 Rodrigo Pinheiro CAMPOS¹, Shuhei SHINZATO², Akio ISHII², Shigenobu OGATA^{2,3}
¹School of Engineering Science, Osaka University, Osaka, 560-8531, Japan, ²Graduate School of Engineering Science, Osaka University, Osaka, 560-8531, Japan, ³Center for Elements Strategy Initiative for Structural Materials, Kyoto University, Kyoto, 606-8501, Japan

A3-11-P04
Dynamics of Rings and Polymer in Polyrotaxane Studied by Molecular Dynamics Simulations and Quasi-Elastic Neutron Scattering Experiments

 Yusuke YASUDA¹, Yuta HIDAKA¹, Koichi MAYUMI¹, Takeshi YAMADA², Kazushi FUJIMOTO³, Susumu OKAZAKI³, Hideaki YOKOYAMA¹, Kohzo ITO¹
¹Department of Advanced Materials Science, School of Frontier Sciences, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8561, Japan, ²Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society (CROSS), IQBRC Bldg., 162-1 Shirakata, Tokai, Naka, Ibaraki 319-1106, Japan, ³Department of Materials Chemistry, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8603, Japan

A3-11-P05
Forecasting of IrO₃ Desorbability from Iridium Alloys by First-Principles Study

 Insung SEO¹, Syunsuke YOKOTA², Yousuke IMAI², Yoshihiro GOHDA¹
¹Tokyo Institute of Technology, ²Ishifuku Metal Industry

A3-11-P06
Effects of Chemical Composition and Surface Reconstruction on Band Alignment of Perovskite Oxides

 Ha-Jun SUNG¹, Yasuhide MOCHIZUKI¹, Fumiyasu OBA^{1,2}
¹Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology, ²Center for Materials Research by Information Integration, Research and Services Division of Materials Data and Integrated System, National Institute for Materials Science

A3-11-P07
***Ab Initio* Local-Energy and Local-Stress Schemes and Application to Metallic Grain Boundaries**

 Masanori KOHYAMA¹, Zhuo XU¹, Shingo TANAKA¹, Yoshinori SHIIHARA²
¹National Institute of Advanced Industrial Science and Technology, ²Toyota Technological Institute

A3-11-P08
Construction of machine learning atomic potential for investigation of lattice defects in BCC iron

 Hideki MORI¹, Taisuke OZAKI²
¹College of Industrial Technology, ²Institute for Solid State Physics, University of Tokyo

A3-11-P09
***Ab initio* approaches for Green's functions of materials using coupled-cluster singles doubles (CCSD)**

Taichi KOSUGI, Yuichiro MATSUSHITA

Tokyo Institute of Technology

A3-11-P10
Stability of Self-Trapped Holes in Ga₂O₃ Polymorphs

 Tomoya GAKE¹, Yu KUMAGAI², Fumiyasu OBA¹
¹Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology, ²Materials Research Center for Element Strategy, Tokyo Institute of Technology

A3-11-P11
First Principles Study For A Quantitative Characterization Of Electrdes Based On Many-Body Hamiltonian

 Shu KANNO¹, Tomofumi TADA¹, Takeru UTSUMI¹, Kazuma NAKAMURA², Hideo HOSONO¹
¹Materials Research Center for Element Strategy, Tokyo Institute of Technology, ²Department of Basic Sciences, Kyushu Institute of Technology

A3-11-P12
Investigation of Au nanoparticles supported on ZnO for CO oxidation using density functional theory

Shih Hsuan HUNG

University of Tokyo

A3-11-P13
Benchmark of Density Functional Theory for Superconductors in Elemental Materials

Mitsuaki KAWAMURA, Taisuke OZAKI

Institute for Solid State Physics, The University of Tokyo

December 11–13, 2019

Symposium A-4

Neutrons for Materials Research

[Organizers]

Toshiji KANAYA (J-PARC MLF, KEK)
 Jun-ichi SUZUKI (CROSS)
 Anna PARADOWSKA (ANSTO)
 Dongfen CHEN (CIAE)

December 11, 2019

Oral Session 1**Interface Science, Slow Dynamics of Polymers**

Time 9:00–11:30 Room Miel-4

Chairpersons Hiroyuki AOKI, Tsukasa MIYAZAKI

A4-11-K01 ▶ Keynote 9:00–9:35

Interfacial Structural Analysis on Polymer Thin Films by
 Neutron Reflectometry

Naoya TORIKAI
 Mie University

A4-11-I02 ▶ Invited 9:35–10:00

Neutron Reflectivity Study of Dynamic Polymer Brush

Hideaki YOKOYAMA
 University of Tokyo

A4-11-I03 ▶ Invited 10:00–10:25

Structure of Model Electrode-electrolyte Interfaces in
 Polymer Electrolyte Fuel Cells and Lithium-ion Batteries

Masashi HARADA¹, Kenji KUDO¹, Hiroyuki KAWAURA¹,
Norifumi L YAMADA²

¹Toyota Central R&D Labs., Inc., ²High Energy Accelerator
 Research Organization

A4-11-I04 ▶ Invited 10:25–10:50

Impact of Solid Interface on Ion Transport in
 Polyelectrolyte Thin Films

Daisuke KAWAGUCHI
 Kyushu University

A4-11-005 10:50–11:10

Structure and Dynamics of Rubbers Reinforced with
 Metallic Diacrylate Studied by Quantum Beams

Toshiji KANAYA
 KEK, J-PARC

A4-11-006 11:10–11:30

Dynamics of Polyrotaxane Glass Investigated by Quasi-
 elastic Neutron Scattering

Koichi MAYUMI¹, Yuta HIDAHA¹, Takeshi YAMADA²,
Masayuki TANIGUCHI¹, Kazuaki KATO^{1,3},
Hideaki YOKOYAMA¹, Tatsuya KIKUCHI⁴, Maiko KOFU⁵,
Kenji NAKAJIMA⁵, Toshiji KANAYA⁵, Kohzo ITO¹

¹The University of Tokyo, ²CROSS, ³NIMS, ⁴Sumitomo
 Rubber Industries, ⁵J-PARC MLF

December 11, 2019

Oral Session 2**Diffraction and Imaging, New Technology**

Time 14:00–15:55 Room Miel-4

Chairperson Kazuya AIZAWA

A4-11-I07 ▶ Invited 14:00–14:25

Development and Applications of the Neutron Grating
 Interferometer for Material Research

Seung Wook LEE
 Pusan National University

A4-11-I08 ▶ Invited 14:25–14:50

Contrast Variation Small Angle Neutron Scattering
 Using Proton Spin Polarization at SANS Spectrometer
 iMATERIA (BL20), J-PARC

Yohei NODA¹, Tomoki MAEDA¹, Takayuki OKU^{1,2},
Satoshi KOIZUMI¹, Tomomi MASUI³, Hiroyuki KISHIMOTO³
¹Ibaraki University, ²J-PARC Center, ³Sumitomo Rubber
 Industries, Ltd.

A4-11-I09 ▶ Invited 14:50–15:15

Structural Response of Piezoelectric Material Studied by
 Stroboscopic Neutron Diffraction under Cyclic Electric
 Field

Takuro KAWASAKI, Stefanus HARJO, Kazuya AIZAWA
 Japan Atomic Energy Agency

A4-11-010 15:15–15:35

Martensitic Transformation in Metastable Steels
 Monitored by Neutron Diffraction

Stefanus HARJO¹, Takuro KAWASAKI¹, Noriyuki TSUCHIDA²,
Satoshi MOROOKA¹, Kazuya AIZAWA¹
¹Japan Atomic Energy Agency, ²University of Hyogo

A4-11-011 15:35–15:55

Observation of Breaking and Recombination of Dihydrogen
 Bonds in Ammonia Borane by High Pressure Neutron
 Diffraction

Satoshi NAKANO¹, Asami SANO-FURUKAWA²,
Takanori HATTORI², Kazuki KOMATSU³, Hiroshi FUJIHISA⁴,
Hiroshi YAMAWAKI⁴, Yoshito GOTOH⁴, Takumi KIKEGAWA⁵
¹National Institute for Materials Science, ²J-PARC Center,
 Japan Atomic Energy Agency, ³University of Tokyo,
⁴National Institute of Advanced Industrial Science and
 Technology, ⁵Institute of Materials Structure Science, High
 Energy Accelerator Research Organization

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 12, 2019

Oral Session 4
Time Division Measurements
Time 9:00–11:15 **Room** Mont-2

Chairperson Jun-ichi SUZUKI

A4-12-K01 ▶ Keynote 9:00–9:35

Stroboscopic Small-angle Neutron Scattering for Metastable Magnetic Skyrmion Lattice in MnSi

Taro NAKAJIMA

The University of Tokyo

A4-12-I02 ▶ Invited 9:35–10:00

Development and Application of Pulsed Magnet System up to 30 Tesla for Neutron Scattering Experiment

 Masao WATANABE¹, Takumi KIHARA², Hiroyuki NOJIRI²
¹J-PARC Center / JAEA, ²Institute for Materials Research / Tohoku University

A4-12-I03 ▶ Invited 10:00–10:25

Study of Deformation Mechanism of Rock Samples Using Simultaneous Measurements of AE Signal and Neutron Diffraction Pattern

 Jun ABE¹, Kotaro SEKINE², Stefanus HARJO³, Takuro KAWASAKI³, Wu GONG⁴, Kazuya AIZAWA³
¹Comprehensive Research Organization for Science and Society (CROSS), ²Japan Oil, Gas and Metals National Corporation (JOGMEC), ³Japan Atomic Energy Agency (JAEA), ⁴Kyoto University

A4-12-I04 ▶ Invited 10:25–10:50

High-Pressure and Temperature Neutron Radiography for Measuring Interdiffusion of H and D in Brucite

 Hiroshi ARIMA¹, Takanori HATTORI², Asami SANO-FURUKAWA², Shinichi MACHIDA¹, Jun ABE¹, Kenichi FUNAKOSHI¹
¹CROSS, ²JAEA

A4-12-I05 ▶ Invited 10:50–11:15

Microstructure of Vanishing Foam Investigated by Time-of-flight at SANS Spectrometer iMATERIA (BL20) J-PARC

 Satoshi KOIZUMI¹, Shiho YADA², Toshikazu YOSHIMURA², Hiroshi SHIMOSEGAWA³, Hiroya FUJITA³, Yukako MATSUE⁴, Yohei NODA¹
¹Ibaraki University, ²Nara Women's University, ³NOF Corporation, ⁴Kracie Home Products, Ltd

December 12, 2019

Oral Session 5
Conduction and Dispersion
Time 14:00–16:15 **Room** Mont-2

Chairperson Yukinobu KAWAKITA

A4-12-K06 ▶ Keynote 14:00–14:35

Structural Study of Hydrides by High Intensity Neutron Total Diffractometer (NOVA)

Kazutaka IKEDA

High Energy Accelerator Research Organization (KEK)

A4-12-I07 ▶ Invited 14:35–15:00

Ion Migration Mechanism for Li₁₀GeP₂S₁₂-type Lithium Conductors Investigated by Neutron Diffraction Measurements

 Satoshi HORI¹, Kota SUZUKI¹, Masaaki HIRAYAMA¹, Ryoji KANNO¹, Takeshi YAJIMA², Zenji HIROI²,

 Yoyo HINUMA³, Takashi OHHARA⁴, Takashi KAMIYAMA⁵
¹Tokyo Institute of Technology, ²University of Tokyo, ³Chiba University, ⁴Japan Atomic Energy Agency, ⁵Institute of Materials Structure Science

A4-12-I08 ▶ Invited 15:00–15:25

Local Structure Analysis on Crystalline Electrode Materials for Rechargeable Batteries by Reverse Monte Carlo Modelling

Naoto KITAMURA

Tokyo University of Science

A4-12-I09 ▶ Invited 15:25–15:50

Insights into Caloric Materials: a Neutron Scattering Study

Bing LI

Institute of Metal Research, Chinese Academy of Sciences

A4-12-I10 ▶ Invited 15:50–16:15

Structure and Dynamic Properties of Water at Extreme Conditions – in a Nano-space and under High Pressures

Koji YOSHIDA, Toshio YAMAGUCHI

Fukuoka University

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 13, 2019

Oral Session 7

Structure and Dynamics of Magnetic and Superconducting Materials

Time 9:00–11:35 Room Miel-5

Chairperson Takashi KAMIYAMA

A4-13-I01 ▶ Invited 9:00–9:25

Combined Neutron Diffraction and X-ray Absorption Spectroscopy Study on the Spin Structures in Cobaltite Double Perovskites

Deok-Yong CHO
Chonbuk National University

A4-13-I02 ▶ Invited 9:25–9:50

Magnetic Structure Analysis Using Z-Rietveld Program

Masato HAGIHALA
High Energy Accelerator Research Organization (KEK)

A4-13-I03 ▶ Invited 9:50–10:15

Development and Application of Magnetic Pair Distribution Function (mPDF) Analysis

Katsuaki KODAMA
Japan Atomic Energy Agency

A4-13-004 10:15–10:35

Neutron Scattering Experiments to Understand the Multiferroicity in the Molecular Magnet $(\text{ND}_4)_2\text{FeCl}_5\cdot\text{D}_2\text{O}$

Javier CAMPO¹, Oscar FABELO²,
Jose Alberto RODRIGUEZ-VELAMAZAN²,
Juan RODRIGUEZ-CARVAJAL², Laurent CHAPON³
¹Aragon Materials Science Institute (CSIC-UZ), ²Institute Laue Langevin, ³Diamond Light Source Ltd

A4-13-005 10:35–10:55

Systematic Study of a New Ferrite Family, 114 Ferrites RBaFe_4O_7 (R = Y, Rare Earth, and etc.) - Neutron Scattering Measurements -

Kazuya KAMAZAWA
Comprehensive Research Organization for Science and Society (CROSS)

A4-13-006 10:55–11:15

Spin Glass Dynamics in a Structural Glass of C4mimFeCl_4

Maiko KOFU¹, Ryuta WATANUKI², Toshiro SAKAKIBARA³,
Seiko OHIRA-KAWAMURA¹, Kenji NAKAJIMA¹,
Takeshi UEKI⁴, Kazuhiro AKUTSU⁵, Osamu YAMAMURO³
¹J-PARC Center, ²Yokohama National University, ³Institute for Solid State Physics, University of Tokyo, ⁴National Institute for Materials Science, ⁵Comprehensive Research Organization for Science and Society

A4-13-007 11:15–11:35

Quantum Dynamics of Hydrogen in Iron-based Superconductor

Jun-ichi YAMAURA
Materials Research Center for Element Strategy, Tokyo Institute of Technology

December 12, 2019

Poster Session

Time 16:30–18:00 Room Trade-0

A4-12-P01

Elastic and Dynamical Structural Properties of La and Mn-doped SrTiO_3 Studied by Neutron Scattering and Their Relation with Thermal Conductivities

Ryoichi KAJIMOTO¹, Mitsutaka NAKAMURA¹, Naoki MURAI¹,
Shin-ichi SHAMOTO¹, Takashi HONDA², Kazutaka IKEDA²,
Toshiya OTOMO², Hiroto HATA³, Takahiro ETO³,
Masaaki NODA⁴, Hideki KUWAHARA⁴, Tetsuji OKUDA³
¹Japan Atomic Energy Agency, ²High Energy Accelerator Research Organization, ³Kagoshima University, ⁴Sophia University

A4-12-P02

Structural Instability-assisted Li-migration in Solid-state Electrolyte $(\text{La,Li})\text{TiO}_3$

Masato MATSUURA¹, Hiroki MORIWAKE²,
Yasuyuki FUJIWARA³, Ryoichi KAJIMOTO⁴,
Mitsutaka NAKAMURA⁴, Koji OHARA⁵,
Yukinobu KAWAKITA⁴

¹Comprehensive Research Organization for Science and Society, ²Nanostructures Research Laboratory, Japan Fine Ceramics Center, ³Faculty of Engineering, Shinshu University, ⁴J-PARC Center, Japan Atomic Energy Agency, ⁵Japan Synchrotron Radiation Research Institute

A4-12-P03

Q-dependence of the Resonance Mode on Iron-based Superconductor $\text{Fe}(\text{Te}_{0.5}\text{Se}_{0.5})$

Motoyuki ISHIKADO¹, Katsuaki KODAMA²,
Ryoichi KAJIMOTO³, Mitsutaka NAKAMURA³,
Yasuhiro INAMURA³, Kazuhiko IKEUCHI¹, Masatoshi ARAI³,
Shin-ichi SHAMOTO⁴

¹CROSS, ²Materials Sciences Research Center, JAEA, ³J-PARC, JAEA, ⁴Advance Science Research Center JAEA

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

A4-12-P04

Semimetal and Superconductivity in Chiral-structure Phase of $R_3T_4Sn_{13}$ ($R = Ce, La$ and $T = Co, Rh, Ir$)

Kazuaki IWASA¹, Yuka OTOMO², Kazuya SUYAMA², Ryoga KARINO¹, Kango MIYAKAWA¹, Seiya NAKAZATO¹, Daisuke HASHIMOTO¹, Mami SHIOZAWA¹, Keitaro KUWAHARA¹, Motoyuki ISHIKADO³, Hajime SAGAYAMA⁴, Hironori NAKAO⁴, Seiko OHIRA-KAWAMURA⁵, Tatsuya KIKUCHI⁵, Kenji NAKAJIMA⁵, Takashi OHHARA⁵, Akiko NAKAO³, Koji MUNAKATA³, Ryoji KIYANAGI⁵, Jean-Michel MIGNOT⁶, Françoise DAMAY⁶, Arsen GUKASOV⁶

¹Ibaraki University, ²Tohoku University, ³Comprehensive Research Organization for Science and Society, ⁴Institute of Materials Structure Science, High Energy Accelerator Research Organization, ⁵J-PARC Center, ⁶Laboratoire Léon Brillouin, CEA-CNRS

A4-12-P05

Monochiral Helimagnetism in Homochiral Crystals of $CsCuCl_3$ Probed by Polarized Neutron Diffraction and Muon Spin Rotation

Kazuki OHISHI¹, Yusuke KOUSAKA², Kazuhisa KAKURAI¹, Jun-ichi SUZUKI¹, Vladimir HUTANU³, Javier CAMPO⁴, Akihiro KODA⁵, Kenji M KOJIMA⁶, Hubertus LUETKENS⁷, Alex AMATO⁷, Katsuya INOUE⁸, Jun AKIMITSU⁹

¹Comprehensive Research Organization for Science and Society (CROSS), ²Osaka Prefecture University, ³RWTH Aachen University and Julich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum, ⁴Aragon Materials Science Institute (CSIC-University of Zaragoza), ⁵High Energy Accelerator Research Organization (KEK), ⁶TRIUMF, ⁷Paul Scherrer Institute, ⁸Hiroshima University, ⁹Okayama University

A4-12-P06

Direct Observation of Ferromagnetic Moment of Potassium Nanoclusters Arrayed in Zeolite A by Polarized Neutron Diffraction

Takehito NAKANO
Ibaraki University

A4-12-P07

Distributions of Water inside Nafion Thin Films on Different Substrates Analyzed by Neutron Reflectometry under Controlled Temperature and Humidity

Teppei KAWAMOTO¹, Makoto AOKI², Taro KIMURA³, Takako MIZUSAWA⁴, Norifumi L. YAMADA⁵, Junpei MIYAKE⁶, Kenji MIYATAKE^{1,6}, Junji INUKAI^{1,6}

¹Fuel Cell Nanomaterials Center, University of Yamanashi, ²Division of Life, Medical, Natural Sciences and Technology, Organization for Advanced and Integrated Research, Kobe University, ³Integrated Graduate School of Medicine, Engineering, and Agricultural Sciences, University of Yamanashi, ⁴Comprehensive Research Organization for Science and Society, ⁵Institute of Materials Structure Science, High Energy Accelerator Research Organization, ⁶Clean Energy Research Center, University of Yamanashi

A4-12-P08

Quasi-elastic and Inelastic Neutron Scattering Spectrometer DNA in MLF, J-PARC and its Application to Materials Science

Yukinobu KAWAKITA¹, Masato MATSUURA², Taiki TOMINAGA², Takeshi YAMADA², Makoto KOBAYASHI², Hiroshi NAKAGAWA¹

¹J-PARC Center, Japan Atomic Energy Agency, ²Comprehensive Research Organization for Science and Society

A4-12-P09

Small and Wide Angle Neutron Scattering Technique for Materials Research

Jun-ichi SUZUKI
Comprehensive Research Organization for Science and Society (CROSS)

A4-12-P10

Current Status of the New Compact Accelerator-based Neutron Facility at AIST

Koichi KINO^{1,2}, Takeshi FUJIWARA^{1,2}, Michihiro FURUSAKA^{1,2}, Noriyosu HAYASHIZAKI^{1,2,3}, Hidetoshi KATO^{1,2}, Ryunosuke KURODA^{1,2}, Koji MICHISHIO^{1,2}, Takemi MUROGA¹, Hiroshi OGAWA^{1,2}, Brian E OROURKE^{1,2}, Nagayasu OSHIMA^{1,2}, Daisuke SATO^{1,2}, Norihiro SEI^{1,2}, Tamao SHISHIDO¹, Ryoichi SUZUKI^{1,2}, Masahito TANAKA^{1,2}, Hiroyuki TOYOKAWA^{1,2}, Akira WATAZU^{1,2}

¹Innovative Structural Materials Association (ISMA), ²National Institute of Advanced Industrial Science and Technology (AIST), ³Tokyo Institute of Technology (Tokyo Tech)

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

Cluster B

New Trend of Materials Research

Symposium

- B-1** Data-Centric Science for Materials Research
- B-2** Materials Integration: Fusion of Materials Science and Experiments through Data Science
- B-3** Mathematical Materials Science
-Mathematical Approaches for Materials Designs in the Data Driven Society-
- B-4** Topological Materials Science for Innovative Functions

December 11–12, 2019

Symposium B-1

Data-Centric Science for Materials Research

[Organizers]

Shinji TSUNEYUKI (Department of Physics, the University of Tokyo)
 Satoshi ITOH (National Institute for Materials Science)
 Fumiyasu OBA (Tokyo Institute of Technology)
 Jason HATTRICK-SIMPERS (National Institute of Standards and Technology)
 Matthias SCHEFFLER (Fritz Haber Institute of the Max Planck Society)
 Jian-xin XIE (University of Science and Technology Beijing)

[Sponsor]


**Science and Technology
of Advanced Materials**

Science and Technology of Advanced Materials(STAM)

December 11, 2019

Oral Session 1

Time 9:00–11:30 Room Miel-1

Chairpersons Shinji TSUNEYUKI, Matthias SCHEFFLER

B1-11-I01 ▶ Invited 9:00–9:30

Data-driven Materials Design and Machine Learning using the Materials Project
Kristin PERSSON

University of California at Berkeley

B1-11-I02 ▶ Invited 9:30–10:00

Building a Foundation for Autonomous Materials Research Systems at an International Scale
Zachary Tim TRAUTT

National Institute of Standards and Technology

B1-11-003 10:00–10:15

Prediction of Material Properties from Its Chemical Formula Using Novel Descriptor “Elemental Fingerprints” with Neural Networks
Jaekyun HWANG¹, Satoshi WATANABE^{1,2}
¹The University of Tokyo, ²National Institute for Materials Science

B1-11-004 10:15–10:30

Structural feature extraction on chemical space by clustering and network analysis
Mariko ITO, Takaaki OHNISHI

The University of Tokyo

B1-11-I05 ▶ Invited 10:30–11:00

Breaking the Curse of Small Data in Materials Informatics
Ryo YOSHIDA

The Institute of Statistical Mathematics

B1-11-006

11:00–11:15

Hybrid Algorithm of Bayesian Optimization and Evolutionary algorithm in Crystal Structure Prediction
Tomoki YAMASHITA^{1,2}, Shinichi KANEHIRA², Nobuya SATO³, Hiori KINO^{1,4}, Koji TSUDA^{1,5,6}, Takashi MIYAKE^{1,3,4}, Tamio OGUCHI^{1,2}
¹Research and Services Division of Materials Data and Integrated System, National Institute for Materials Science, ²Institute of Scientific and Industrial Research, Osaka University, ³Research Center for Computational Design of Advanced Functional Materials, National Institute of Advanced Industrial Science and Technology, ⁴Elements Strategy Initiative Center for Magnetic Materials, National Institute for Materials Science, ⁵Graduate school of Frontier Sciences, The University of Tokyo, ⁶RIKEN Center for Advanced Intelligence Project

B1-11-007

11:15–11:30

Fast Prediction of Crystal Structure Stability by Machine Learning
Yuki INADA

The University of Tokyo

December 11, 2019

Oral Session 2

Time 14:00–16:00 Room Miel-1

Chairpersons Satoshi ITOH, Youhei YAMAJI

B1-11-I08 ▶ Invited

14:00–14:30

Verification and Error Estimates for *Ab Initio* Data
Claudia DRAXL

HU Berlin

B1-11-009

14:30–14:45

High-Throughput Calculations and Machine-Learning Prediction of Oxygen Vacancy Formation Energies
Yu KUMAGAI¹, Akira TAKAHASHI², Fumiyasu OBA^{1,2,3}
¹Materials Research Center for Element Strategy, Tokyo Institute of Technology, ²Laboratory for Materials and Structures, Tokyo Institute of Technology, ³CMI2, MaDIS, National Institute for Materials Science

B1-11-010

14:45–15:00

Machine learning and ab initio calculations for proton-conducting oxides
Yoshihiro YAMAZAKI

Kyushu University

B1-11-I11 ▶ Invited

15:00–15:30

Unavoidable Disorder and Entropy in Multi-Component Systems
Stefano CURTAROLO

Center of Materials Genomics, Duke University

B1-11-012

15:30–15:45

Systematic generation of tight-binding Hamiltonians for ferromagnets and its application
Takashi KORETSUNE

Tohoku University

B1-11-013 15:45–16:00

Construction of Neutral Network Potential to Investigate Interface Structures of Au(111)/Li₃PO₄Koji SHIMIZU¹, Wei LIU¹, Wenwen LI², Yasunobu ANDO², Emi MINAMITANI³, Satoshi WATANABE^{1,4}¹The University of Tokyo, ²National Institute of Advanced Industrial Science and Technology, ³Institute for Molecular Science, ⁴National Institute for Materials Science

December 11, 2019

Oral Session 3

Time 16:30–18:30 Room Miel-1

Chairpersons Yu KUMAGAI, Takashi KORETSUNE

B1-11-114 ▶ Invited 16:30–17:00

Screening materials from high-throughput ab initio calculations and machine learning

Gian-Marco RIGNANESE

Université catholique de Louvain

B1-11-015 17:00–17:15

Discovery of Oxide Ion Conductors by ensemble-scope descriptor

Nobuko OHBA, Seiji KAJITA, Akitoshi SUZUMURA, Shin TAJIMA, Ryoji ASAHI

Toyota Central R&D Laboratories Inc.

B1-11-016 17:15–17:30

Computational screening of novel solid electrolyte candidates for all-solid-state battery by high-throughput DFT and data science techniquesRandy JALEM¹, Yoshitaka TATEYAMA^{1,2,4}, Ichiro TAKEUCHI^{2,5}, Masanobu NAKAYAMA^{1,2,4,5}¹Center for Green Research on Energy and Environmental Materials & Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN), National Institute for Materials Science (NIMS), Tsukuba, Japan,²Center for Materials research by Information Integration (CMI²), Research and Services Division of Materials Data and Integrated System (MaDIS), NIMS, Tsukuba, Japan,³PRESTO, Japan Science and Technology Agency (JST), Saitama, Japan, ⁴Elements Strategy Initiative for Catalysts & Batteries, Kyoto University, Kyoto, Japan, ⁵Nagoya Institute of Technology (NITech), Nagoya, Japan

B1-11-117 ▶ Invited 17:30–18:00

Data-Driven Computational Design of Emerging Microstructural Material Systems

Wei CHEN

Northwestern University

B1-11-018 18:00–18:15

Origin of High-Temperature Superconductivity Revealed by Boltzmann MachineYouhei YAMAJI¹, Teppei YOSHIDA², Atsushi FUJIMORI³, Masatoshi IMADA^{3,4}¹The University of Tokyo, ²Kyoto University, ³Waseda University, ⁴Toyota Physical and Chemical Research Institute

B1-11-019 18:15–18:30

Design of oil molecules by high-throughput molecular dynamics simulationsSeiji KAJITA, Tomoyuki KINJO, Tomoki NISHI
Toyota Central R&D Labs., Inc.

December 12, 2019

Oral Session 6

Time 16:30–18:30 Room Port-1

Chairpersons Fumiyasu OBA, Isao OHKUBO

B1-12-101 ▶ Invited 16:30–17:00

Machine learning assisted composition design of Copper-base alloys with high strength and high electrical conductivityHuadong FU, Hongtao ZHANG, Jianxin XIE
University of Science and Technology Beijing

B1-12-002 17:00–17:15

Development of layered complex nitrides accelerated by the combination of first-principles calculation, machine learning, and experimentsIsao OHKUBO, Takao MORI
National Institute for Materials Science (NIMS)

B1-12-003 17:15–17:30

Understanding of diffraction pattern and homology in disordered materialsYohei ONODERA^{1,2}, Shinji KOHARA^{3,2,4,5}, Shuta TAHARA^{6,2}, Atsunobu MASUNO^{7,2}, Hiroyuki INOUE⁸, Motoki SHIGA^{5,9,16}, Akihiko HIRATA^{10,11,12,13}, Koichi TSUCHIYA¹⁴, Yasuaki HIRAOKA^{15,2,13}, Ippei OBAYASHI^{16,13}, Koji OHARA¹⁷, Osami SAKATA³¹Institute for Integration Radiation and Nuclear Science, Kyoto University, ²Center for Materials research by Information Integration (CMI²), Research and Services Division of Materials Data and Integrated System (MaDIS), National Institute for Materials Science (NIMS), ³Research Center for Advanced Measurement and Characterization, NIMS, ⁴Research and Utilization Division, Japan Synchrotron Radiation Research Institute, ⁵PRESTO, Japan Science and Technology Agency, ⁶Faculty of Science, University of the Ryukyus, ⁷Graduate School of Science and Technology, Hiroasaki University, ⁸Institute of Industrial Science, The University of Tokyo, ⁹Department of Electrical, Electronic and Computer Engineering, Faculty of Engineering, Gifu University, ¹⁰Graduate School of Fundamental Science and Engineering, Waseda University, ¹¹Kagami Memorial Research Institute for Materials Science and Technology, Waseda University, ¹²Mathematics for Advanced Materials-OIL, AIST-Tohoku University, ¹³WPI Advanced Institute for Materials Research, Tohoku University, ¹⁴Design and Producing Field, Corrosion Resistant Alloy Group, Research Center for Structural Materials, NIMS, ¹⁵Kyoto University Institute for Advanced Study, Kyoto University, ¹⁶Center for Advanced Intelligence Project, RIKEN, ¹⁷Diffraction and Scattering Division, Center for Synchrotron Radiation Research, Japan Synchrotron Radiation Research Institute

B1-12-I04 ▶ Invited 17:30–18:00

Data-Driven Science for X-Ray Absorption Fine Structure Spectra Measured in Synchrotron Radiation Facilities
Ichiro AKAI^{1,2}, Yoshiki SENO², Masaichiro MIZUMAKI³, Toru AONISHI⁴
¹Kumamoto University, ²Kyushu Synchrotron Light Research Center, ³Japan Synchrotron Radiation Research Institute, ⁴Tokyo Institute of Technology

B1-12-005 18:00–18:15

Sparse modeling of extended x-ray absorption fine structures (EXAFS)
Yasuhiko IGARASHI^{1,2,3}, Hiroyuki SETOYAMA⁴, Toshihiro OKAJIMA⁴, Ichiro AKAI^{4,5}, Masato OKADA^{1,3}
¹Graduate School of Frontier Science, The University of Tokyo, ²Japan Science and Technology Agency, PRESTO, ³Research and Services Division of Materials Data and Integrated System, National Institute for Material Science, ⁴Kyushu Synchrotron Light Research Center, ⁵Institute of Pulsed Power Science, Kumamoto University, Kumamoto

B1-12-006 18:15–18:30

Statistical Machine Learning for Spectrum Imaging Data Analysis
Motoki SHIGA^{1,2,3}, Shunsuke MUTO⁴
¹Gifu University, ²Japan Science and Technology Agency, ³RIKEN, ⁴Nagoya University

December 12, 2019

Poster Session
Time 14:00–15:30 **Room** Trade-0

B1-12-P01
Descriptor for Efficient Crystal Structure Prediction Using the Bayesian Optimization
Nobuya SATO¹, Tomoki YAMASHITA^{2,3}, Tamio OGUCHI^{2,3}, Koji HUKUSHIMA^{2,4}, Takashi MIYAKE^{1,2}
¹National Institute of Advanced Industrial Science and Technology, ²National Institute for Materials Science, ³Institute of Scientific and Industrial Research, Osaka University, ⁴Department of Basic Science, University of Tokyo

B1-12-P02
Testing Procedure Anomaly Detection Method for Materials Big Data
Peng SHI, Zhen ZHAO

University of Science and Technology Beijing

B1-12-P03
Predicted High-yield Synthesis Of Manganese-oxide Nanosheets Through Exfoliation Of The Layered Composites
Kyohei NODA¹, Yasuhiko IGARASHI^{2,3}, Hiroaki IMAI¹, Yuya OAKI^{1,3}
¹Keio University, ²The University of Tokyo, ³JST PRESTO

B1-12-P04
Crystal structure simulation by assimilating incomplete experimental data
Seiji YOSHIKAWA¹, Naoto TSUJIMOTO¹, Daiki ADACHI¹, Ryosuke AKASHI¹, Syngye TODO^{1,2,3}, Shinji TSUNEYUKI^{1,2}
¹Department of Physics, The University of Tokyo, ²Institute for Solid State Physics, The University of Tokyo, ³Research and Services Division of Materials Data and Integrated System, National Institute for Materials Science

B1-12-P05
3D Phase-Field Modeling of Solid-State Sintering: The Diffusion Mechanism Dependence of Grain-Boundary Formation
Yuki OKADA, Akiyasu YAMAMOTO, Akimitsu ISHII, Akinori YAMANAKA

Tokyo University of Agriculture and Technology

B1-12-P06
Modeling the normal-state current transport in iron-based superconducting polycrystalline materials
Takuya OBARA, Akiyasu YAMAMOTO

Tokyo University of Agriculture and Technology

B1-12-P07
Prediction of X-ray Absorption Spectra from Crystal Structures: Machine Learning Approaches
Hidekazu IKENO^{1,2}, Naoyuki MIYAMOTO¹
¹Osaka Prefecture University, ²PRESTO, JST

B1-12-P08
Deep Neural Network Approach to the X-ray Absorption Spectroscopy
Naoyuki MIYAMOTO¹, Hidekazu IKENO^{1,2}
¹Department of Materials Science, Osaka Prefecture University, ²Precursory Research for Embryonic Science and Technology (PRESTO), Japan Science and Technology Agency (JST)

B1-12-P09
Uncovering new stable Fe-Nd-X structures with machine learning
Duong Nguyen NGUYEN

Japan Advanced Institute of Science and Technology

B1-12-P10
Machine-Learning Guided Discovery of a New Thermoelectric Material
Yuma IWASAKI

NEC

B1-12-P11**Machine-Learned Kinetic Energy Functional in Isolated Systems and its Combination with Orbital-Free Density Functional Theory**

Junji SEINO^{1,2}, Ryo KAGEYAMA³, Mikito FUJINAMI³,
Yasuhiro IKABATA¹, Hiromi NAKAI^{1,3,4}

¹Waseda Research Institute for Science and Engineering, Waseda University, ²PRESTO, Japan Science and Technology Agency, ³School of Advanced Science and Engineering, Waseda University, ⁴ESICB, Kyoto University

B1-12-P12**Machine-Learning-Assisted Exploration for Novel Lanthanide Based Metal-Organic Frameworks**

Yu KITAMURA¹, Daisuke TANAKA^{1,2}

¹Kwansei Gakuin University, ²JST PRESTO

B1-12-P13**Novel Material Search Method of Lithium Ion Conductors Using Machine Learning**

Kota SUZUKI^{1,2}, Kosei OHURA¹, Atsuto SEKO^{2,3},
Masaaki HIRAYAMA¹, Isao TANAKA³, Ryoji KANNO¹

¹Tokyo Institute of Technology, ²JST, PRESTO, ³Kyoto University

B1-12-P14**First-principles prediction of magnetic structures in crystal**

Michi-To SUZUKI

Institute for Materials Research

B1-12-P15**Machine Learning Assisted Synthesis of Novel Coordination Polymer**

Takuma WAKIYA¹, Yoshinobu KAMAKURA¹,
Daisuke TANAKA^{1,2}

¹Kwansei Gakuin University, ²JST PRESTO

B1-12-P16**Machine learning quantum Monte Carlo simulations for strongly correlated electron materials**

Naoto TSUJI

RIKEN Center for Emergent Matter Science (CEMS)

B1-12-P17**Prediction of Fibrinogen Adsorption on Self-Assembled Monolayers (SAM) from Chemical Structures and Quantification of Structures' Importance using Artificial Neural Network (ANN)**

Rudolf JASON¹, Hayashi TOMOHIRO^{1,2}

¹Tokyo Institute of Technology, ²JST-PRESTO

B1-12-P18**AI-Robot-driven Materials Research for Inorganic Materials**

Ryota SHIMIZU^{1,2}, Shigeru KOBAYASHI¹, Yasunobu ANDO³,
Taro HITOSUGI¹

¹Tokyo Institute of Technology, ²PRESTO, Japan Science and Technology Agency, ³National Institute of Advanced Industrial Science and Technology

B1-12-P19**Machine Learning-Based Analysis for High-throughput Peak Detection in Synchrotron X-ray Spectromicroscopy**

Naoka NAGAMURA¹, Tarojiro MATSUMURA³,
Shotaro AKAHO³, Kenji NAGATA^{1,2}, Yasunobu ANDO³

¹National Institute of Materials Science, ²Japan Science and Technology Agency, PRESTO, ³National Institute of Advanced Industrial Science and Technology

B1-12-P20**Material Parameter Estimation for Phase-field Simulation of Solid-state Sintering using Data Assimilation**

Akinori YAMANAKA¹, Akimitsu ISHII¹, Yuki OKADA¹,
Yusuke SHIMADA², Akiyasu YAMAMOTO¹

¹Tokyo University of Agriculture and Technology, ²Tohoku University

B1-12-P21**First-Principles Study and Descriptor Selection of Site Preference of Hydride Anions in Hexagonal BaVO_{3-x}H_x**

Kazuki SHITARA^{1,2,3}, Takafumi YAMAMOTO⁴,
Hiroshi KAGEYAMA⁵, Hiroki MORIWAKE^{2,3},
Akihide KUWABARA^{2,3}

¹Joint and Welding Research Institute, Osaka University, ²Nanostructures Research Laboratory, Japan Fine Ceramics Center, ³Laboratory for Materials and Structures, Tokyo Institute of Technology, ⁴Graduate School of Engineering, Kyoto University

B1-12-P22**Development of thermophysical property database for materials informatics**

Tetsuya BABA, Erina FUJITA, Yibin XU

National Institute for Materials Science

December 12–13, 2019

Symposium B-2

Materials Integration: Fusion of Materials Science and Experiments through Data Science

[Organizers]

Junya INOUE (The University of Tokyo)
Irina ROSLYAKOVA (Ruhr-Universität Bochum)
Masahiko DEMURA (National Institute for Materials Science)

December 12, 2019

Oral Session 5

Time 14:00–16:10 Room Port-3

Chairperson Junya INOUE

B2-12-K01 ▶ Keynote 14:00–14:40

3-D Phase-Field Simulations to machine-learn 3-D Features from 2-D Microstructures

Ingo STEINBACH, Mansur AHMED, Muhammad Adil ALI, Irina ROSLYAKOVA
Ruhr University Bochum

B2-12-I02 ▶ Invited 14:40–15:10

Network Theory Meets Materials Science

Christopher WOLVERTON¹, Vinay HEGDE¹, Murat AYKOL²
¹Northwestern University, ²Toyota Research Institute

B2-12-I03 ▶ Invited 15:10–15:40

Data management for atomistic simulation: design and case studies

Yury LYSOGORSKIY, Thomas HAMMERSCHMIDT, Matous MROVEC, Ralf DRAUTZ
Ruhr University Bochum

B2-12-I04 ▶ Invited 15:40–16:10

Workflow control APIs for inverse problem analysis

Satoshi MINAMOTO¹, Kaita ITO¹, Takuya KADOHIRA¹, Junya INOUE^{1,2}, Masahiko DEMURA¹
¹National Institute for Materials Science, ²The University of Tokyo

December 12, 2019

Oral Session 6

Time 16:30–18:20 Room Port-3

Chairperson Masahiko DEMURA

B2-12-I05 ▶ Invited 16:30–17:00

On the consideration of inverse problem analysis for performance of structural materials

Manabu ENOKI
The University of Tokyo

B2-12-I06 ▶ Invited 17:00–17:30

Artificial Materials Intelligence

Irina ROSLYAKOVA
Ruhr University Bochum

B2-12-I07 ▶ Invited 17:30–18:00

Accelerating Materials Innovation: ICME, Materials Design, Data and the Underlying Workforce Training

E. Begum GULSOY¹, Juan J. DE PABLO², Gregory B. OLSON¹, Peter W. VOORHEES¹
¹Northwestern University, ²University of Chicago

B2-12-008 18:00–18:20

Starrydata: an open database of published plot data for materials informatics

Yukari KATSURA
The University of Tokyo

December 13, 2019

Oral Session 7

Time 9:30–11:30 Room Port-3

Chairperson Makoto WATANABE

B2-13-K01 ▶ Keynote 9:30–10:10

Data-scientific Approaches in Materials Integration

Masahiko DEMURA
National Institute for Materials Science

B2-13-002 10:10–10:30

Physical-based data-driven modeling strategy for creep behavior of Co-base superalloys

Setareh ZOMORODPHOOSH, Irina ROSLYAKOVA, Ingo STEINBACH
Ruhr University Bochum

B2-13-003 10:30–10:50

Prediction of Creep Rupture Time for Weld Joints of 2 1/4Cr-1Mo Steel

Hitoshi IZUNO¹, Masahiko DEMURA¹, Masayoshi YAMAZAKI¹, Masaaki TABUCHI², Daisuke ABE³, Keisuke TORIGATA³
¹Research and Services Division of Materials Data and Integrated System (MaDIS), National Institute for Materials Science (NIMS), ²Research Center for Structural Materials, National Institute for Materials Science (NIMS), ³Corporate Research & Development, IHI Corporation

B2-13-004 10:50–11:10

Universal Framework of Bayesian Creep Model Selection for Steel

Yoh-ichi MOTOTAKE¹, Hitoshi IZUNO², Kenji NAGATA², Masahiko DEMURA², Masato OKADA³
¹Institute of Statistical Mathematics, ²National Institute for Materials Science, ³University of Tokyo

B2-13-005

11:10–11:30

Identification of the transformation kinetics of steels from a dilatometric curve using a machine learning method

Hoheok KIM¹, Junya INOUE^{1,2}, Masato OKADA³, Kenji NAGATA³

¹Graduate School of Materials Engineering, The University of Tokyo, ²Research Center for Advanced Science and Technology, The University of Tokyo, ³Graduate School of Frontier Science, The University of Tokyo

December 13, 2019

Oral Session 8

Time 14:00–15:50 Room Port-3

Chairperson Satoshi MINAMOTO

B2-13-I06

► Invited

14:00–14:30

PRISMS-Plasticity: An Open-Source Crystal Plasticity Finite Element Software

Mohammadreza YAGHOUBI¹, Sriram GANESAN^{2,6}, Srihari SUNDAR², Aaditya LAKSHMANAN², Aeriel MURPHY-LEONARD^{1,5}, Shiva RUDRARAJU^{3,4}, John E. ALLISON¹, Veera SUNDARARAGHAVAN²

¹Materials Science and Engineering, University of Michigan, Ann Arbor, ²Aerospace Engineering, University of Michigan, Ann Arbor, ³Mechanical Engineering, University of Michigan, Ann Arbor, MI, ⁴Mechanical Engineering, University of Wisconsin-Madison, WI, ⁵U.S. Naval Research Laboratory, Washington, DC, ⁶Intel, Hillsboro, OR

B2-13-007

14:30–14:50

Observation and crystal plasticity simulation of microstructurally short crack propagation in rolled Ti-6Al-4V alloy

Fabien BRIFFOD, Takayuki SHIRAIWA, Manabu ENOKI
The University of Tokyo

B2-13-008

14:50–15:10

Prediction of defect-induced fatigue failures using physical model and data assimilation techniques

Takayuki SHIRAIWA, Ryota SAKAGUCHI, Fabien BRIFFOD, Pornthep CHIVAVIBUL, Manabu ENOKI
The University of Tokyo

B2-13-009

15:10–15:30

Observation of fatigue crack initiation and crystal plasticity analysis of flame-resistant Mg alloy

Seiya NAKAJIMA
University of Tokyo

B2-13-010

15:30–15:50

Autonomous generation of process-structure linkages for two-phase composites from simulation data obtained from micromechanical finite element models

A.F. MARSHALL, Surya R. KALIDINDI
Georgia Institute of Technology

December 13, 2019

Oral Session 9

Time 16:30–18:30 Room Port-3

Chairperson Manabu ENOKI

B2-13-I11

► Invited

16:30–17:00

Materials Integration for Carbon Fiber reinforced composites

Tomonaga OKABE¹
¹Tohoku University, ²University of Washington

B2-13-012

17:00–17:20

Evaluation of Reduction of Stress Concentration around a Circular Hole by Fiber Steering Placement Technique

Hiroshi SUEMASU, Yuichiro AOKI
Japan Aerospace Exploration Agency

B2-13-013

17:20–17:40

Simulation of Phase Separated Polymer Matrix for an Applicatoin to a Composite

Yutaka OYA¹, Naofumi UMEMOTO¹, Tomonaga OKABE¹, Toshihiro KAWAKATSU²
¹Department of Aerospace Engineering, Tohoku University, ²Department of Physics, Tohoku University

B2-13-I14

► Invited

17:40–18:10

Materials Integration for powder-based metal manufacturing processes

Makoto WATANABE^{1,2}
¹National Institute for Materials Science, ²Research Center for Advanced Science and Technology, The University of Tokyo

B2-13-015

18:10–18:30

Image analysis tensile test method at elevated temperature to obtain true stress-true strain curves up to large strain in Ti alloy

Shiro TORIZUKA
University of Hyogo

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 11–13, 2019

Symposium B-3

Mathematical Materials Science
-Mathematical Approaches for Materials
Designs in the Data Driven Society-

[Organizers]

Motoko KOTANI (Tohoku University)
Kazuto AKAGI (Tohoku University)
Yasumasa NISHIURA (Tohoku University)
Shin'ichi OISHI (Waseda University)
Stephen Hyde (Australian National University)
Christian Ratsch (UCLA)

December 11, 2019

Oral Session 1

Time 9:00–11:20 Room Work-3

 Opening
9:00–9:10

B3-11-K01 ▶ Keynote 9:10–9:40

Mathematics in Topological Materials for Quantum Computing

Zhenghan WANG
Microsoft Station Q and UCSB

B3-11-002 9:40–10:00

Crystallographic T-duality as the Baum-Connes isomorphism

Yosuke KUBOTA
RIKEN

B3-11-003 10:00–10:20

 Anomaly Matching and Symmetry-protected Critical Phases in $SU(N)$ Spin Systems in 1+1 Dimensions

 Yuan YAO¹, Chang-Tse HSIEH^{1,2}, Masaki OSHIKAWA¹
¹Institute for Solid State Physics, Univ. of Tokyo, ²Kavli Institute for the Physics and Mathematics of the Universe

 Break
10:20–10:30

B3-11-I04 ▶ Invited 10:30–11:00

Neural network as a discrete geometry for materials through holographic principle

Koji HASHIMOTO
Osaka University

B3-11-005 11:00–11:20

Nuclear states and spectra in holographic QCD

 Koji HASHIMOTO¹, Yoshinori MATSUO¹, Takeshi MORITA^{2,3}
¹Department of Physics, Osaka University, ²Department of Physics, Shizuoka University, ³Graduate School of Science and Technology, Shizuoka University

December 11, 2019

Oral Session 2

Time 14:00–16:00 Room Work-3

B3-11-K06 ▶ Keynote 14:00–14:30

The Atiyah-Patodi-Singer index theorem and domain walls

Mikio FURUTA
University of Tokyo

B3-11-007 14:30–14:50

Second-order topological phases realized by chiral symmetry

Ryo OKUGAWA
Tohoku University

B3-11-008 14:50–15:10

A Generalized Boundary Condition Applied on Lieb-Schultz-Mattis Type Incompatibilities and Many-body Chern Numbers

 Yuan YAO, Masaki OSHIKAWA
Institute for Solid State Physics, University of Tokyo

B3-11-009 15:10–15:30

Emergent Flat Bands in Fermionic Honeycomb Networks

Chenhua GENG
Institute for Solid State Physics, University of Tokyo

 Break
15:30–15:40

B3-11-010 15:40–16:00

Synchronized Dynamics of Carbon Nanotubes Dispersed in Solution

Masahito SANO
Yamagata University

December 11, 2019

Oral Session 3**Time** 16:30–18:40 **Room** Work-3**B3-11-111** ▶ Invited 16:30–17:00**Structure-Property Relationship of Heterogeneous Elastomers Investigated by Network Centrality**Yoshifumi AMAMOTO¹, Ken KOJIO³, Atsushi TAKAHARA³, Yuichi MASUBUCHI², Takaaki OHNISHI¹¹The University of Tokyo, ²Nagoya University, ³Kyushu University**B3-11-012** 17:00–17:20**Smooth Dependence with Respect to Delay: Temporal Order of Reaction**Junya NISHIGUCHI

Tohoku University

B3-11-013 17:20–17:40**Model Selection of Phase-Field Crystal Models for Targeted Crystalline Patterns**Natsuhiko YOSHINAGA

Tohoku University

B3-11-014 17:40–18:00**Study of Grain Boundary Structures using Topological Data Analysis and Simple Evaluation with Local Energy**Fumiko OGUSHI

National Institute for Materials Science

B3-11-015 18:00–18:20**Topological data analysis of the magnetic domain for the automated visualization of the origin of coercivity**Masato KOTSUGI¹, Takumi YAMADA^{1,2}, Yuta SUZUKI¹, Chiharu MITSUMATA², Kanta ONO^{2,3}, Tetsuro UENO⁴, Ippey OBAYASHI^{5,6}, Kazuto AKAGI^{2,5}, Yasuaki HIRAOKA^{2,5,6,7}¹Tokyo University of Science, ²MI2I-NIMS, ³High Energy Accelerator Research Organization(KEK), ⁴National Institutes for Quantum and Radiological Science and Technology (QST), ⁵Tohoku Univ. AIMR, ⁶RIKEN AIP, ⁷Kyoto Univ. KUIAS**B3-11-016** 18:20–18:40**Fractal dimension, persistent homology dimension, and fractal dynamics in the terahertz region: the case of protein lysozyme**Tatsuya MORI¹, Yasuhiro FUJII², Suguru KITANI³, Yohei YAMAMOTO¹, Kentaro SHIRAKI¹, Akitoshi KOREEDA², Seiji KOJIMA¹¹University of Tsukuba, ²Ritsumeikan University, ³Tokyo Institute of Technology

December 12, 2019

Oral Session 6**Time** 16:30–18:30 **Room** Port-2**B3-12-K01** ▶ Keynote 16:30–17:00**Machine-Learned Interatomic Potentials For Alloy Modeling**Gus Lewis Warren HART

Brigham Young University

B3-12-I02 ▶ Invited 17:00–17:30**Optimization Problems in Data Driven Science -Fundamentals and Applications in Materials Informatics-**Akihisa ICHIKI

Nagoya University

B3-12-003 17:30–17:50**Applied-math approaches for filler-filled polymer nanocomposites**Katsumi HAGITA

National Defense Academy

B3-12-004 17:50–18:10**Natural Computing with Light-Activated Colloidal Crystals**Toshiharu SAIKI¹, Okuto IKEDA¹, Yuka TAKAMATSU¹, Bokusui NAKAYAMA¹, Eiji YAMAMOTO¹, Masashi KUWAHARA²¹Keio University, ²National Institute of Advanced Industrial Science and Technology**B3-12-005** 18:10–18:30**Developments of Molecular Spin Gyroids**Kunio AWAGA

Nagoya University

December 13, 2019

Oral Session 7**Time** 9:30–11:40 **Room** Port-2**B3-13-K01** ▶ Keynote 9:30–10:00**Soft Crystals: Minimal Froths versus Generalized Quantizers**Gregory GRASON

University of Massachusetts Amherst

B3-13-I02 ▶ Invited 10:00–10:30**Computational Study of the Microphase-Separated Structure and Elastic Property of Block Copolymers**Takeshi AOYAGI

National Institute of Advanced Industrial Science and Technology

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

B3-13-003 10:30–10:50

Modeling of Entangled Polymer Dynamics
Yuichi MASUBUCHI, Takashi UNEYAMA
Nagoya University

B3-13-I04 ▶ Invited 10:50–11:20

3-Dimensional Topology and Poly-continuous Pattern
Koya SHIMOKAWA
Saitama University

B3-13-005 11:20–11:40

Rouse Dynamics of Topological Polymers and Polymer Networks Through Gaussian Random Graph Embeddings
Tetsuo DEGUCHI
Ochanomizu University

December 13, 2019

Oral Session 8

Time 14:00–15:50 Room Port-2

B3-13-I06 ▶ Invited 14:00–14:30

Carbon Structures and a Discrete Surface Theory
Hisashi NAITO¹, Toshiaki OMORI², Chen TAO³,
Motoko KOTANI⁴
¹Graduate School of Mathematics, Nagoya University,
²Cifra Co., Ltd, ³Mathematical Institute, Tohoku University,
⁴AIMR, Tohoku University

B3-13-007 14:30–14:50

Eigenvalues of the Laplacian on the Goldberg-Coxeter Constructions for 3- and 4-valent Graphs
Toshiaki OMORI¹, Hisashi NAITO², Tatsuya TATE³
¹Cifra Co., Ltd., ²Nagoya University, ³Tohoku University

B3-13-008 14:50–15:10

Mathematically-designed graphene in electrochemical water splitting
Yoshikazu ITO
University of Tsukuba

B3-13-009 15:10–15:30

Bond Twist and Curvature in Three-Dimensional Carbon Networks
Andreas DECHANT
Advanced Institute for Materials Research, Tohoku University

B3-13-010 15:30–15:50

Mathematical Approach for Molecular Conduction
Yuta TSUJI, Kazunari YOSHIZAWA
Kyushu University

December 13, 2019

Oral Session 9

Time 16:30–18:00 Room Port-2

B3-13-I11 ▶ Invited 16:30–17:00

Challenge with mathematics to fabricate microstructures using minimal surfaces
Seiichi TAKAMI¹, Rikuto TAKAI¹, Toshiaki TAIRA²,
Akira ENDO²
¹Nagoya University, ²National Institute of Advanced
Industrial Science and Technology

B3-13-012 17:00–17:20

Variational problem for anisotropic surface energy
Miyuki KOISO, Yoshiki JIKUMARU
Kyushu University

B3-13-013 17:20–17:40

Comparison inequalities on directed graphs under a lower Ollivier Ricci curvature bound
Yohei SAKURAI
Tohoku University

B3-13-014 17:40–18:00

Development of Metal Coordinate Surfactants (MCSs) as Functional Nanomaterials
Toshiaki TAIRA, Tomohiro IMURA, Akira ENDO
National Institute of Advanced Industrial Science and
Technology

December 12, 2019

Poster Session

Time 14:00–15:30 Room Trade-0

B3-12-P01

Gapless states on topological defects
Minoru ETO
Yamagata University

B3-12-P02

Nanoscale Heat Engines Based on Magnon-Phonon Coupled States
Koji SATO
Tohoku University

B3-12-P03

First-principles study of the Chern insulator induced by spin chirality
Hikaru SAWAHATA¹, Naoya YAMAGUCHI¹, Fumiyuki ISHII²
¹Graduate School of Natural Science and Technology,
Kanazawa University, ²Nanomaterials Research Institute,
Kanazawa University

B3-12-P04**Photocleavable Regenerative Star Poly(dimethyl siloxane) Networks for the Tuning of Viscoelasticity**

Satoshi HONDA, Minami OKA, Taro TOYOTA
The University of Tokyo

B3-12-P05**Rheology of Cholesteric Blue Phases**

Shuji FUJII
Hokkaido University

B3-12-P06**Physical Implementation of Swarm Intelligence in Colloidal Particle Systems**

Bokusui NAKAYAMA¹, Toshiharu SAIKI¹, Eiji YAMAMOTO¹,
Masashi KUWAHARA²
¹Keio University, ²National Institute of Advanced Industrial
Science and Technology

B3-12-P07**Upgrade Design of the Diffractometer for Small Angle Scattering using tender X-ray at BL-15A2 at the Photon Factory**

Hideaki TAKAGI¹, Noriyuki IGARASHI¹, Yasuko NAGATANI¹,
Hiromasa OHTA², Nobutaka SHIMIZU¹
¹High Energy Accelerator Organization, ²Mitsubishi Electric
System & Service Co., Ltd

B3-12-P08**Fluid Mechanical Duality for Minimal Surfaces in Euclidean Space and Maximal Surfaces in Spacetime**

Shintaro AKAMINE
Nagoya University

B3-12-P09**Graphene Encapsulation Effects on NiMo Alloy in Oxygen Evolution Reaction**

Samuel JEONG¹, Kailong HU¹, Tatsuhiko OHTO²,
Yuki NAGATA³, Hideki MASUDA¹, Jun-ichi FUJITA¹,
Yoshikazu ITO^{1,4}
¹University of Tsukuba, ²Osaka University, ³Max Plank
Institute, ⁴PRESTO

B3-12-P10**Preparation of Metal-Organic Framework Templated Carbons and Applications to Electrode Materials**

Hirofumi YOSHIKAWA
Kwansei Gakuin University

B3-12-P11**Topological Data Analysis of Amorphous Carbon at High-Temperature**

Kazuto AKAGI
Tohoku University

December 11, 2019

Symposium B-4

Topological Materials Science for Innovative Functions

[Organizer]

Shuichi MURAKAMI (Tokyo Institute of Technology)

[Sponsor]


 国立研究開発法人 科学技術振興機構
 Japan Science and Technology Agency

December 11, 2019

Oral Session 1

Time 9:00–11:30 Room Work-8

Chairperson Akio KIMURA

Preparation

9:00–9:20

B4-11-001 9:20–9:40

Anomalous dielectric response in insulators with the π Zak phase

 Shuichi MURAKAMI¹, Motoaki HIRAYAMA², Yusuke AIHARA¹
¹Tokyo Institute of Technology, ²RIKEN

B4-11-002 9:40–10:00

Symmetry indicators for topological superconductors

 Haruki WATANABE
 University of Tokyo

B4-11-I03 ▶ Invited 10:00–10:30

Real-space recipes of topological crystalline states

 Chen FANG
 Chinese Academy of Sciences

B4-11-004 10:30–10:50

Variants of symmetry-based indicators in the band theory

 Ken SHIOZAKI
 Kyoto University

B4-11-005 10:50–11:10

Electrides as a New Platform of Topological Materials

 Motoaki HIRAYAMA¹, Satoru MATSUI², Hideo HOSONO²,
 Shuichi MURAKAMI³
¹RIKEN, Center for Emergent Matter Science, ²Materials Research Center for Element Strategy, Tokyo Institute of Technology, ³Department of Physics, Tokyo Institute of Technology

B4-11-006 11:10–11:30

Predicting topological materials by symmetry-based indicators

 Tiantian ZHANG^{1,2}
¹Institute of Physics, CAS, ²Tokyo Institute of Technology

December 11, 2019

Oral Session 2

Time 14:00–16:00 Room Work-8

Chairperson Motoaki HIRAYAMA

B4-11-I07 ▶ Invited 14:00–14:30

Incorporating Magnetism into Topological Materials for Innovative Functions

 Akio KIMURA
 Hiroshima University

B4-11-008 14:30–14:50

Flexible Hall sensor using the anomalous Hall effect of nanocrystalline Fe-Sn films

 Kohei FUJIWARA¹, Yosuke SATAKE¹, Junichi SHIOGAI¹,
 Takeshi SEKI^{1,2}, Atsushi TSUKAZAKI^{1,2}
¹IMR, Tohoku University, ²CSRN, Tohoku University

B4-11-009 14:50–15:10

High-resolution angle-resolved photoemission study of topological heterostructures

 Kosuke NAKAYAMA
 Tohoku University

B4-11-I10 ▶ Invited 15:10–15:40

Exploring Topological States Coupled to Charge Density Wave

 Kyoko ISHIZAKA
 The University of Tokyo

B4-11-011 15:40–16:00

Ab initio calculation of surface states and ARPES of Weyl semimetal candidate material MoTe₂

 Ryota ONO¹, Alberto MARMODORO², Jan MINÁR³,
 Yoshitaka NAKATA¹, Hubert EBERT², Jürgen BRAUN²,
 Kazuyuki SAKAMOTO⁴, Peter KRÜGER¹
¹Chiba University, ²Ludwig-Maximilians-Universität München, ³University of West Bohemia, ⁴Osaka University

December 11, 2019

Oral Session 3**Time** 16:30–18:30 **Room** Work-8Chairperson Shuichi MURAKAMI

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

B4-11-012 16:30–16:50**Quantized Surface Transport Observed in Cd₃As₂ Films**Masaki UCHIDA^{1,2}, Shinichi NISHIHAYA¹, Yusuke NAKAZAWA¹, Ryosuke KURIHARA³, Kazuto AKIBA³, Markus KRIENER⁴, Atsushi MIYAKE³, Yasujiro TAGUCHI⁴, Masashi TOKUNAGA³, Masashi KAWASAKI^{1,4}¹Department of Applied Physics, University of Tokyo,²PRESTO, JST, ³ISSP, University of Tokyo, ⁴RIKEN CEMS**B4-11-113** ▶ Invited 16:50–17:20**Topological Properties of Complex Magnetic Materials from Ab-Initio Theory**Jan-Philipp HANKE

Peter Gruenberg Institut, Forschungszentrum Juelich

B4-11-014 17:20–17:40**Magnetic skyrmions in centrosymmetric materials**Shinichiro SEKI

University of Tokyo

B4-11-115 ▶ Invited 17:40–18:10**Exploration of Topological Quantum Materials**Takao SASAGAWA

Tokyo Institute of Technology

B4-11-016 18:10–18:30**Single Crystal Thin Films of Three-Dimensional Topological Insulators via Non-catalytic Vapor Phase Epitaxial Crystal Growth and Applications**Katsumi TANIGAKI, Yu Stephane MATSUSHITA,Khuong K. HUYNH

Tohoku University

December 11, 2019

Poster Session**Time** 19:00–20:30 **Room** Trade-0**B4-11-P01****Helicoid and Catenoid Surfaces in a Liquid Crystalline Dimer Driven by Surface Tension**Khoa LE

Tokyo University of Science

B4-11-P02**Chirality Imaging Using X-ray Wave Front With Topological Defects**Yoshiki KOHMURA¹, Kei SAWADA¹, Masaichiro MIZUMAKI², Kenji OHWADA³, Tetsu WATANUKI³, Tetsuya ISHIKAWA¹¹RIKEN, ²Japan Synchrotron Radiation Research Institute,³National Institutes for Quantum and Radiological Science and Technology (QST)

Cluster C

Novel Structural Materials Based on New Principles

Symposium

- C-1** Fundamental Issues of Structural Materials
- C-2** Mille-feuille Structured Light-weight Materials
- C-3** Hard and Tough Ceramics
- C-4** Tough Polymers

December 11–12, 2019

Symposium C-1

Fundamental Issues of Structural Materials

[Organizers]

Isao TANAKA (Kyoto University)
 Haruyuki INUI (Kyoto University)
 Nobuhiro TSUJI (Kyoto University)

Hyoung Seop KIM (Pohang University of Science and Technology)
 Guillaume LAPLANCHE (Ruhr-Universität Bochum)

December 11, 2019

Oral Session 1

Time 9:00–11:20 **Room** Mont-1

Chairpersons Nobuhiro TSUJI, Cem TASAN

C1-11-K01 ▶ Keynote 9:00–9:40

Overcoming the limits of the TRIP-effect utilizing reverse transformations

Cem TASAN, Shaolou WEI
 Department of Materials Science and Engineering,
 Massachusetts Institute of Technology

C1-11-002 9:40–10:00

Preferential Ultra Fine Grain Formation in Harmonic Structure Designed SUS304L Austenitic Stainless Steel

Kei AMEYAMA¹, Masashi NAKATANI², Bhupendra SHARMA¹,
Mie KAWABATA¹

¹Department of Mechanical Engineering, Faculty of Science and Engineering, Ritsumeikan University, ²Graduate School of Science and Engineering, Ritsumeikan University

Break
10:00–10:10

C1-11-I03 ▶ Invited 10:10–10:40

Multiple Strengthening and Microstructure Optimization of Heterostructured High-Entropy Alloy

Hyoung Seop KIM
 Department of Materials Science and Engineering, Pohang University of Science and Technology

C1-11-004 10:40–11:00

Effect Of Microalloying On Microstructure And Mechanical Properties Of Cast Al_{0.6}CoCrFeNi Compositionally Complex Alloys.

Alex ASABRE¹, Aleksander KOSTKA²,
Janine PFETZING-MICKLICH², Oleg STRYZHYBORODA³,
Ulrike HECHT³, Guillaume LAPLANCHE¹

¹Ruhr-Universität Bochum (RUB), Bochum, D-44780, Germany, ²Zentrum für Grenzflächendominierte Höchstleistungswerkstoffe (ZGH), RUB, Bochum D-44780, Germany, ³ACCESS e.V., Aachen, D-52072, Germany

C1-11-005 11:00–11:20

In-situ characterization of heterogeneous deformation behavior in a Fe-Ni-C alloy using neutron diffraction, DIC and thermography

Wu GONG^{1,2}, Stefanus HARJO², Wenqi MAO³,
Takayuki YAMASHITA², Nobuhiro TSUJI^{1,3}

¹Elements Strategy Initiative for Structural Materials, Kyoto University, ²J-PARC Center, Japan Atomic Energy Agency, ³Department of Materials Science and Engineering, Kyoto University

December 11, 2019

Oral Session 2

Time 14:00–16:10 **Room** Mont-1

Chairpersons Haruyuki INUI, John LEWANDOWSKI

C1-11-K06 ▶ Keynote 14:00–14:40

Pressure/Stress State Effects on Fundamental Mechanisms of Plastic Deformation in Structural Materials

John LEWANDOWSKI
 Department of Materials Science and Engineering, Case Western Reserve University

C1-11-I07 ▶ Invited 14:40–15:10

The Atomic Structure and Dynamic Behavior of Twinning Dislocation of Rhombohedral Twinning in α -Al₂O₃

Eita TOCHIGI¹, Bin MIAO¹, Naoya SHIBATA^{1,2},
Yuichi IKUHARA^{1,2,3}

¹Institute of Engineering Innovation, The University of Tokyo, ²Japan Fine Ceramic Center, ³ESISM, Kyoto University

Break
15:10–15:20

C1-11-I08 ▶ Invited 15:20–15:50

Room Temperature Deformation Behavior of Hard Intermetallic Compounds Investigated by Micropillar Compression Method

Kyosuke KISHIDA, Haruyuki INUI
 Department of Materials Science and Engineering, Kyoto University

C1-11-009 15:50–16:10

Interdiffusion In Quaternary Cr-Fe-Co-Ni High-Entropy Alloys

Adeline DURAND¹, Linqing PENG^{2,3}, Ying YANG²,
Guillaume LAPLANCHE¹, James R MORRIS^{2,4},
Gunther EGGELER¹, Easo P GEORGE^{2,4}

¹Institut für Werkstoffe, Ruhr-Universität Bochum (RUB), ²Materials Science and Technology Division, Oak Ridge National Laboratory, ³Grinnell College, Iowa, ⁴Department of Materials Science and Engineering, University of Tennessee

December 11, 2019

Oral Session 3**Time** 16:30–18:30 **Room** Mont-1Chairpersons Kyosuke KISHIDA, Guillaume LAPLANCHE**C1-11-I10** ▶ **Invited** 16:30–17:00**Kinetics of phase decomposition in high-entropy alloys and effects on mechanical properties**Guillaume LAPLANCHE¹, Sondre BERGLUND¹,
Christian REINHART¹, Aleksander KOSTKA²,
Easo P. GEORGE^{3,4}¹Institut für Werkstoffe, Ruhr-Universität Bochum, ²Zentrum für Grenzflächendominierte Höchstleistungswerkstoffe (ZGH), Ruhr-Universität Bochum, ³Materials Science and Technology Division, Oak Ridge National Laboratory, ⁴Department of Materials Science and Engineering, University of Tennessee**C1-11-011** 17:00–17:20**Deformation behavior and microstructure evolution in equi-atomic CoCrFeMnNi high-entropy alloy highly deformed by torsion at elevated temperatures**Reza GHOLIZADEH¹, Yu BAI^{1,2}, Akinobu SHIBATA^{1,2},
Nobuhiro TSUJI^{1,2}¹Department of Materials Science & Engineering, Kyoto University, ²ESISM (Elements Strategy Initiative for Structural Materials), Kyoto University

<div style="display: flex; align-items: center; justify-content: center;"> <div style="font-size: 3em; margin-right: 10px;">[</div> <div style="text-align: center;"> <p>Break</p> <p>17:20–17:30</p> </div> <div style="font-size: 3em; margin-left: 10px;">]</div> </div>
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C1-11-012 17:30–17:50**Microstructure and mechanical properties of equimolar TiZrNbHfTa High-Entropy Alloy Prepared via Powder Metallurgy**Bhupendra SHARMA¹, Eri AKADA², Naoto TOGAWA²,
Mie KAWABATA³, Kei AMEYAMA³¹Ritsumeikan University Research Organization of Science and Technology, Kusatsu City, 525-8577, Japan, ²Graduate School of Science and Engineering, Ritsumeikan University, Kusatsu City, 525-8577, Japan, ³Faculty of Science and Engineering, Ritsumeikan University, Kusatsu City, 525-8577, Japan**C1-11-013** 17:50–18:10**Formation of the thermal vacancy in high entropy alloys**Taichi ABE¹, Ikuo OHNUMA¹, Toshiyuki KOYAMA²¹Research Center for Structural Materials, National Institute for Materials Science, ²Department of Materials Design Innovation Engineering, Graduate School of Engineering, Nagoya University**C1-11-014** 18:10–18:30**Experimental determination and thermodynamic evaluation of Cr-Mn-Ni system**Katsunari OIKAWA

Department of Metallurgy, Graduate School of Engineering, Tohoku University

December 12, 2019

Oral Session 4**Time** 9:00–11:20 **Room** Mont-1Chairpersons Shigenobu OGATA, Yunzhi WANG**C1-12-K01** ▶ **Keynote** 9:00–9:40**Uncovering the deformation mechanisms of ordered intermetallic phases in Ni-base superalloys**Yunzhi WANG

Department of Materials Science and Engineering, The Ohio State University

C1-12-002 9:40–10:00**Deformation mechanism and mechanical properties of mixed amorphous-crystalline system through atomic simulations**Tomotsugu SHIMOKAWA

Department of Mechanical Systems Engineering, Kanazawa University

<div style="display: flex; align-items: center; justify-content: center;"> <div style="font-size: 3em; margin-right: 10px;">[</div> <div style="text-align: center;"> <p>Break</p> <p>10:00–10:10</p> </div> <div style="font-size: 3em; margin-left: 10px;">]</div> </div>
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C1-12-I03 ▶ **Invited** 10:10–10:40**Modeling of pop-ins in nanoindentation**Shigenobu OGATA^{1,2}, Takahito OHMURA^{3,2}, Yuji SATO¹,
Shuhei SHINZATO¹¹Graduate School of Engineering Science, Osaka University, ²ESISM, Kyoto University, ³National Institute for Materials Science**C1-12-004** 10:40–11:00**Bidirectional Stability Breaking in Thermodynamic Average for Multicomponent Alloys**Koretaka YUGE

Department of Materials Science and Engineering, Kyoto University

C1-12-005 11:00–11:20**Reactive Molecular Dynamics Simulation of Intergranular Stress Corrosion Cracking Process of FeNiCr-based High Entropy Alloy**Narumasa MIYAZAKI, Chang LIU, Qian CHEN,
Momoji KUBO

Institute for Materials Research, Tohoku University

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 12, 2019

Oral Session 5
Time 14:00–15:55 **Room** Mont-1

Chairperson Takahito OHMURA

C1-12-006 14:00–14:15

Microscopic mechanism of hydrogen-related fracture in 2Mn-0.1C steel with ferrite microstructure

 Kazuho OKADA¹, Akinobu SIBATA^{1,2}, Wu GONG^{2,3}, Nobuhiro TSUJI^{1,2}
¹Department of Materials Science and Engineering, Kyoto University, ²Elements Strategy Initiative for Structural Materials (ESISM), Kyoto University, ³J-PARC Center, Japan Atomic Energy Agency

C1-12-007 14:15–14:30

Effect of serration on deformation behavior in high-Mn austenitic steel

 SUK YOUNG HWANG¹, Myeong-Heom PARK², Yu BAI¹, Akinobu SHIBATA^{1,2}, Nobuhiro TSUJI^{1,2}
¹Department of Materials Science and Engineering, Kyoto University, ²Elements Strategy Initiative for Structural Materials (ESISM), Kyoto University

C1-12-008 14:30–14:45

Microstructural origin of high work-hardenability in ultrafine-grained CoCrNi medium entropy alloy

 Shuhei YOSHIDA¹, Genki YAMASHITA¹, Takuto IKEUCHI¹, Yu BAI^{1,2}, Akinobu SHIBATA^{1,2}, Nobuhiro TSUJI^{1,2}
¹Department of Materials Science and Engineering, Kyoto University, ²Element Strategy Initiative for Structural Materials (ESISM), Kyoto University

C1-12-009 14:45–15:00

Mechanical properties and strengthening mechanism of ultrafine grained Al-Mg alloys

 Xiaodong LAN¹, Si GAO¹, Myeong-heom PARK^{1,2}, Akinobu SHIBATA^{1,2}, Nobuhiro TSUJI^{1,2}
¹Department of Materials Science and Engineering, Kyoto University, ²Element Strategy Initiative for Structural Materials (ESISM), Kyoto University

 Break
15:00–15:10

C1-12-010 15:10–15:25

Influence of Deformation Temperature on Mechanical Properties of Harmonic Structure Designed SUS316L Austenitic Stainless Steel

 Koki YAGI¹, Masashi NAKATANI¹, Bhupendra SHARMA², Mie KAWABATA³, Cinzia MENAPACE⁴, Kei AMEYAMA³
¹Graduate School of Science and Engineering, Ritsumeikan University, ²Ritsumeikan University Research Organization of Science and Technology, ³Faculty of Science and Engineering, Ritsumeikan University, ⁴Faculty of Industrial Engineering, University of Trento

C1-12-011 15:25–15:40

Harmonic Structure Design of Fe-0.3wt% Carbon Steel with Outstanding Strength and Toughness

 Ryohei IRITANI¹, Kenta HORI¹, Bhupendra SHARMA², Mie KAWABATA³, Kei AMEYAMA³
¹Graduate School of Science and Engineering, Ritsumeikan University, Kusatsu City, 525-8577, Japan., ²Ritsumeikan University Research Organization of Science and Technology, Kusatsu City, 525-8577, Japan., ³Faculty of Science and Engineering, Ritsumeikan University, Kusatsu City, 525-8577, Japan.

C1-12-012 15:40–15:55

Mechanical Properties of Harmonic Structure Designed CrMnFeCoNi High Entropy Alloy

 Naoto TOGAWA¹, Bhupendra SHARMA², Zhang ZHE³, Mie KAWABATA⁴, Xu CHEN³, Kei AMEYAMA⁴
¹Graduate School of Science and Engineering, Ritsumeikan University, Kusatsu City, 5258577, Japan, ²Ritsumeikan University Research Organization of Science and Technology, Kusatsu City, 5258577, Japan, ³Tianjin University, Tianjin, 300072, China, ⁴Facility of Science and Engineering, Ritsumeikan University, Kusatsu City, 5258577, Japan

December 12, 2019

Oral Session 6
Time 16:30–17:30 **Room** Mont-1

Chairperson Kaneaki TSUZAKI

C1-12-013 16:30–16:45

Unique deformation structure evolution in a harmonic structure designed Ti-24Nb-25Zr alloy

 Kentaro NAGANO¹, Sharma BHUPENDRA², Mie KAWABATA³, Kei AMEYAMA³
¹Ritsumeikan University of Mechanical Engineering, ²Ritsumeikan University Research Organization of Science and Technology, ³Faculty of Mechanical Engineering, Ritsumeikan University

C1-12-014 16:45–17:00

Influences of Multi-Thermo-Mechanical Process on Ti Harmonic Structured compacts

 Akito SHIMAMURA¹, Motoki MIYAKOSHI¹, Bhupendra SHARMA², Mie KAWABATA³, Kei AMEYAMA³
¹Graduate School of Science and Engineering, Ritsumeikan University, Japan, ²Ritsumeikan University Research Organization of Science and Technology, Japan, ³Faculty of Science and Engineering, Ritsumeikan University, Japan

C1-12-015 17:00–17:15

Effect of Thermo-mechanical Processing on Fatigue Properties of Commercially Pure Titanium with Harmonic Structure

 Kohei OSAKI¹, Shoichi KIKUCHI², Yoshikazu NAKAI¹, Mie KAWABATA³, Kei AMEYAMA³
¹Department of Mechanical Engineering, Graduate School of Engineering, Kobe University, ²Department of Mechanical Engineering, Faculty of Engineering, Shizuoka University, ³Department of Mechanical Engineering, Faculty of Science and Engineering, Ritsumeikan University

C1-12-016

17:15–17:30

Effect of Microstructures on Mechanical and Electrical Properties of Aluminum-Carbon Nanotube (Al-CNT) composites

Kazuaki AOI¹, Fumio OGAWA², Mie KAWABATA²,
Takamoto ITOH², Kei AMEYAMA²

¹Graduate school of Science and Engineering, Ritsumeikan University, ²College of Science and Engineering, Ritsumeikan University

C1-11-P07

Excellent Mechanical Behavior with Anomalous Glassy State of High-Pressure Heat-Treated Zr-Based Bulk Metallic Glass

Yasuto ABE¹, Rui YAMADA², Yuki SHIBAZAKI³,
Wookha RYU², Junji SAIDA²

¹Graduate School of Engineering, Tohoku University, ²Frontier Research Institute for Interdisciplinary Sciences (FRIS), Tohoku University, ³National Institute for Materials Science (NIMS)

December 11, 2019

Poster Session

Time 19:00–20:30 **Room** Trade-0

C1-11-P01

The Coadsorption Effect of Cl⁻ and H₂O on the Various Defect Al₂O₃ Film Surface

Chuan-Hui ZHANG

University of Science and Technology Beijing

C1-11-P02

Overcoming the strength-ductility trade-off dilemma in TRIP-assisted multiphase steel with lean alloy composition

Avala LAVAKUMAR

Kyoto University

C1-11-P03

Effect of Texture Change on Strain-Induced Martensitic Transformation of Semi-Austenitic Stainless Steel SUS304

Taku MATSUO, Tatsuya GOTOH, Kyoichi ISHIDA,
Muneyuki IMAFUKU

Tokyo City University

C1-11-P04

Influence of Atomic Size Difference on Dislocation Emission from Grain Boundaries in High-Entropy Alloys

Kohei SHIOTANI, Tomoaki NIYAMA,
Tomotsugu SHIMOKAWA

Kanazawa University

C1-11-P05

Study of thermodynamic stability of HEA alloy using first principles calculation

Masanori ENOKI, Hiroshi OHTANI

Institute of Multidisciplinary Research for Advanced Materials, Tohoku University

C1-11-P06

Vacancy migration behavior in a CoCrFeMnNi high entropy alloy

Kazuki SUGITA¹, Ryusei OGAWA¹, Masataka MIZUNO¹,
Hideki ARAKI¹, Atsushi YABUUCHI², Atsushi KINOMURA²

¹Graduate School of Engineering, Osaka University,
²Institute for Integrated Radiation and Nuclear Science, Kyoto University

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 12–13, 2019

Symposium C-2

Mille-feuille Structured Light-weight Materials

[Organizers]

Eiji ABE (University of Tokyo)
 Yoshihito KAWAMURA (Kumamoto University)
 Hiromu SAITO (Tokyo University of Agriculture and Technology)

December 12, 2019

Oral Session 4

Time 9:00–11:30 Room Work-8

Chairperson Eiji ABE

C2-12-001 9:00–9:30

Strengthening of Mg-based LPSO-phase alloys induced by the formation of deformation kink band, and its development to other Mille-feuille structured materials

Koji HAGIHARA¹, Michiaki YAMASAKI²,
 Yoshihito KAWAMURA², Takayoshi NAKANO¹

¹Osaka University, ²Magnesium Research Center & Department of Materials Science, Kumamoto University

C2-12-002 9:30–9:50

Fatigue in Extruded Mg/LPSO two-phase alloys: a Combined Experimental-Numerical Study

Fabien BRIFFOD, Takayuki SHIRAIWA, Manabu ENOKI
 The University of Tokyo

C2-12-003 9:50–10:10

Hardness properties and microstructures of caliber rolled Mg-Y-Zn alloy

Hidetoshi SOMEKAWA¹, Daisuke ANDO²

¹National Institute for Materials Science, ²Tohoku University

Break
 10:10–10:20

C2-12-004 10:20–10:50

Influence of Multimodal Microstructure Evolution on Corrosion Behavior of Extruded Mg-Zn-Y Alloys with Mille-feuille Structure of α -Mg and LPSO phases

Michiaki YAMASAKI¹, Tomohiro KAWAKAMI¹, Zhiming SHI²,
 Andrej ATRENS², Yoshihito KAWAMURA¹

¹Kumamoto University, ²The University of Queensland

C2-12-005 10:50–11:10

Effects of Pre-Straining and Heat-Treatment on Compression Strength in a Directionally Solidified Long Period Stacking Ordered Type Mg-Zn-Y Alloy

Mayumi SUZUKI¹, Tatsuya YAMAGUCHI², Yuki TAKAHASHI³,
 Koji HAGIHARA⁴

¹Toyama Prefectural University, ²Graduate Student, Toyama Prefectural University, ³Undergraduate Student, Toyama Prefectural University (Now with Toyama Murata Manufacturing Co., Ltd), ⁴Department of Adaptive Machine Systems, Graduate School of Engineering, Osaka University

C2-12-006 11:10–11:30

In Situ Neutron Diffraction during Compression or Tension of Mg₉₇Zn₁Y₂ consisting of LPSO phase and α Mg phase

Stefanus HARJO¹, Kazuya AIZAWA¹, Wu GONG^{1,2},
 Takuro KAWASAKI¹

¹Japan Atomic Energy Agency, ²Kyoto University

December 12, 2019

Oral Session 5

Time 14:00–16:00 Room Work-8

Chairperson Toshiyuki FUJII

C2-12-007 14:00–14:30

Formation and Annihilation of Disclination in Kink Microstructure

Tomonari INAMURA
 Tokyo Institute of Technology

C2-12-008 14:30–15:00

FTMP-based Descriptions of Rotational Field Evolutions

Tadashi HASEBE
 Kobe University

C2-12-009 15:00–15:20

FTMP-based Kink Deformation and Strengthening Mechanisms for Mille-feuille Structures

Yuta NAWA, Tadashi HASEBE
 Kobe University

C2-12-010 15:20–15:40

Solute Segregation at Kink Boundaries in Mille-feuille Structured Mg Alloys

Daisuke EGUSA¹, Eiji ABE^{1,2}

¹The University of Tokyo, ²National Institute for Materials Science

C2-12-011 15:40–16:00

Mechanical Properties of two-phase Nb-TiNi alloys with Mille-feuille Structure

Kazuhiro ISHIKAWA¹, Toyoaki SUZUKI², Kiyoshi AOKI²
¹Kanazawa University, ²Kitami Institute of Technology

December 13, 2019

Oral Session 7

Time 9:00–11:30 Room Work-8

Chairperson Hiromu SAITO

C2-13-001 9:00–9:30

Nanostructure control of organic-silica nanocomposite by using block copolymers as templates

Reiko SAITO

Tokyo Institute of Technology

C2-13-002 9:30–9:50

Lamellar Microdomain Structures of Liquid Crystal Block Copolymers under Uniaxial Elongation

Masatoshi TOKITA, Jumpei KURIBAYASHI

Tokyo Institute of Technology

C2-13-003 9:50–10:10

Fabrication and Mechanical Properties of Metal Flake Particles/Epoxy Resin Composite

Takashi KUROSE, Yurato SAKO, Hiroshi ITO

Yamagata University

C2-13-004 10:10–10:30

Depth-resolved nanostructure analysis of thin block copolymer films undergoing microphase separation examined by tender X-rays

Hiroshi OKUDA¹, Shin-ichi SAKURAI², Noriyuki IGARASHI³, Nobutaka SHIMIZU³, Yusuke TAMENORI⁴, Michiaki YAMASAKI⁵, Yoshihito KAWAMURA⁵¹Kyoto University, ²Kyoto Inst. Technol., ³KEK PF, ⁴JASRI, ⁵Kumamoto University

C2-13-005 10:30–10:50

The origin of structural stability and solute clustering in Mg-M-Y (M= Ni, Cu, Co, and Zn) alloys with long-period stacking ordered structure

Takao TSUMURAYA¹, Tamio OGUCHI²¹Magnesium Research Center, Kumamoto University, ²Institute of Scientific and Industrial Research, Osaka University

C2-13-006 10:50–11:10

Local Structural Analysis of Mille-feuille Structured Mg-Zn-Y Alloy using X-ray Fluorescence Holography

Koji KIMURA¹, Takumi NISHIOKA¹, Yuta YAMAMOTO¹, Koji HAGIHARA², Hitoshi IZUNO³, Naohisa HAPPO⁴, Shinya HOSOKAWA⁵, Eiji ABE⁶, Motohiro SUZUKI⁷, Tomohiro MATSUSHITA⁷, Kouichi HAYASHI¹¹Nagoya Institute of Technology, ²Osaka University, ³National Institute for Materials Science, ⁴Hiroshima City University, ⁵Kumamoto University, ⁶The University of Tokyo, ⁷Japan Synchrotron Radiation Research Institute

C2-13-007

11:10–11:30

Microstructure Evolution of MgYTM (TM=Zn,Cu,Ni) glass ribbons under constant rate heating

Hiroshi OKUDA¹, Mikihito ITO¹, Shan LIN¹, Michiaki YAMASAKI², Yoshihito KAWAMURA²¹Kyoto University, ²Kumamoto University

December 12, 2019

Poster Session

Time 16:30–18:00 Room Trade-0

C2-12-P01

High-Strength Polymer through a Microstructure Control

Kentaro MUKUMOTO¹, Koji OKUMA², Daisuke EGUSA¹, Hiromu SAITO², Eiji ABE^{1,3}¹The Univ. of Tokyo, ²Tokyo University of Agriculture and Technology, ³National Institute for Material Science

C2-12-P02

Hybrid *in situ* neutron diffraction of Mg-based 18R LPSO alloy under compressive deformationKazuya AIZAWA¹, Wu GONG², Stefanus HARJO¹, Takuro KAWASAKI¹¹Japan Atomic Energy Agency, ²Kyoto University

C2-12-P03

Nanostructure distribution analysis in multilayered aluminum alloys by combined use of scalar tomography and scanning small-angle scattering

Shan LIN¹, Hiroshi OKUDA¹, Yukihito NISHIKAWA²¹Kyoto University, ²Kyoto Inst. Technol. Kyoto

C2-12-P04

Local Strains around Kinks in Mille-feuille Structured Mg Alloys

Yutaka URAKAWA¹, Daisuke EGUSA¹, Mitsuhiro ITAKURA², Eiji ABE^{1,3}¹The University of Tokyo, ²Japan Atomic Energy Agency, ³National Institute for Material Science

C2-12-P05

Two-directional Micro-Laue Diffraction Mapping under Compression for Investigation of Kink Deformation Behavior in LPSO Mg Alloys

Shigeru KIMURA, Kazushi SUMITANI, Kentaro KAJIWARA
Japan Synchrotron Radiation Research Institute

C2-12-P06

Dependence of Vickers Hardness on Layer Thickness in Electrodeposited Ni-Co-Cu / Cu Multilayered Films

Hiroyuki HAGIWARA
Osaka City University

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I



Symposium A

C2-12-P07

Influence of microstructure evolution on fracture toughness of a rapidly solidified ribbon-consolidated Mg-Zn-Y-Al alloy

Soya NISHIMOTO¹, Michiaki YAMASAKI², Shin-ichi INOUE², Yoshihito KAWAMURA²

¹Graduate Student, Graduate School of Science and Technology, Kumamoto University, ²Magnesium Research Center/Department of Materials Science, Kumamoto University

Symposium B

C2-12-P08

Study on the Two-phase Materials with Mille-feuille Structures with a Stacking of Hard and Soft Phases

Atsushi ISHIZAKA
Hokkaido University

Symposium C

C2-12-P09

Evaluation Of The Relationship Between Internal Structures And Mechanical Properties In Multilayer Films

Yuki WATANABE¹, Akira ISHIGAMI¹, Shoutaro NISHITUJI¹, Takashi KUROSE², Hiroshi ITO^{1,2}

¹Yamagata University, ²Reserch Center for GREEN Materials and Advanced Prosessing (GMAP)

Symposium D

C2-12-P10

Localized Deformation of Electrodeposited Ni-Co-Cu/Cu Multilayered Films Subjected to Compressive Straining

Yoshihisa KANEKO
Osaka City University

Symposium E

C2-12-P11

Preparation and Mechanical Properties of Metal Flake Particles/Epoxy Resin Composites

Yutaro SAKO, Takashi KUROSE, Hiroshi ITO
Yamagata University

Symposium F

Symposium G

Symposium H

Symposium I

December 11–13, 2019

Symposium C-3

Hard and Tough Ceramics

[Organizers]

Junichi TATAMI (Yokohama National University)
Norimasa NISHIYAMA (Tokyo Institute of Technology)
Satoshi KITAOKA (Japan Fine Ceramics Center)
Fumihiko WAKAI (Tokyo Institute of Technology)

December 11, 2019

Oral Session 2

Time 14:00–16:05 Room Work-6

Chairperson Norimasa NISHIYAMA

C3-11-I01 ▶ Invited 14:00–14:30

Size Dependent Hardness and Mechanical Energy Accommodation in Nanocrystalline Ceramics

James WOLLMERSHAUSER, Boris FEIGELSON,
Heonjune RYOU, Edward GORZKOWSKI, Kathryn WAHL
U.S. Naval Research Laboratory

C3-11-I02 ▶ Invited 14:30–14:55

Synthesis of Transparent Nano-ceramics under Ultrahigh Pressure

Tetsuo IRIFUNE
Geodynamics Research Center, Ehime University

C3-11-I03 ▶ Invited 14:55–15:20

Continuous Strengthening in Nanotwinned Diamond

Bo XU
Yanshan University

C3-11-I04 ▶ Invited 15:20–15:45

Nanopolycrystalline diamond: strength and mechanisms of plastic deformation

Yanbin WANG¹, Feng SHI¹, Hiroaki OHFUJI², Julien GASC¹,
Norimasa NISHIYAMA³, Tony YU¹, Toru SHINMEI²,
Tetsuo IRIFUNE²

¹CARS, Univ Chicago, ²GRC, Ehime Univ, ³LMS, Institute of Innovative Research, TIT

C3-11-005 15:45–16:05

Mechanical properties of transparent birefringent aluminosilicate nanoceramics

Nico Alexander GAIDA^{1,2}, Norimasa NISHIYAMA³,
Oliver BEERMANN⁴, Atsunobu MASUNO⁵,
Ulrich SCHÜRMAN², Christopher GIEHL⁴, Ken NIWA¹,
Masashi HASEGAWA¹, Shrikant BHAT⁶, Robert FARLA⁶,
Lorenz KIENLE²

¹Department of Materials Physics, Nagoya University,
²Institute for Materials Science, Kiel University, ³Laboratory for Materials and Structures, Tokyo Institute of Technology,
⁴Institute of Geosciences, Kiel University, ⁵Graduate School of Science and Technology, Hirosaki University, ⁶Deutsches Elektronen-Synchrotron (DESY)

December 11, 2019

Oral Session 3

Time 16:30–18:25 Room Work-6

Chairperson James WOLLMERSHAUSER

C3-11-I06 ▶ Invited 16:30–16:55

Highly Distinctive Mechanical Properties of Ultrafine Nano-polycrystalline Diamond and cBN

Hitoshi SUMIYA
Sumitomo Electric Industries, Ltd.

C3-11-I07 ▶ Invited 16:55–17:20

Complex atomic structure and three-dimensional single dopant distribution in Ce-doped cubic boron nitride

Ryo ISHIKAWA^{1,2}, Naoya SHIBATA^{1,3}, Takashi TANIGUCHI³,
Yuichi IKUHARA^{1,3}

¹University of Tokyo, ²JST PRESTO, ³Japan Fine Ceramics Center, ⁴National Institute for Materials Science

C3-11-I08 ▶ Invited 17:20–17:45

Crack-resistant and High Elastic Modulus Oxide Glasses Prepared by a Levitation Technique

Atsunobu MASUNO
Hirosaki University

C3-11-009 17:45–18:05

Fabrication of Transparent Ceramics by Colloidal Processing and SPS

Tohru S. SUZUKI
National Institute for Materials Science

C3-11-010 18:05–18:25

Nanopolycrystalline β -Si₃N₄ and γ -Si₃N₄: their mechanical and physical properties

Norimasa NISHIYAMA, Fumihiko WAKAI
Tokyo Institute of Technology

December 12, 2019

Oral Session 4

Time 9:00–11:25 Room Work-6

Chairpersons Jun-ichi TATAMI, Koji MORITA

C3-12-K01 ▶ Keynote 9:00–9:30

Polymer-Derived Ceramics --- 40 Years of Research and Innovation in Advanced Ceramics

Ralf Peter RIEDEL
TU Darmstadt

C3-12-I02 ▶ Invited 9:30–9:55

Novel Metal Nitrides Synthesized under High Pressures - Compression Behaviors, Crystal Chemistry and Electronic States -

Masashi HASEGAWA
Nagoya University

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

C3-12-003 9:55–10:15
High-pressure Synthesis of Nitride Hard-materials.
Fumio KAWAMURA, Hitoshi YUSA, Takashi TANIGUCHI
 National Institute for Materials Science

[Break
10:15–10:25]

C3-12-004 10:25–10:45
High pressure synthesis and compression behavior of hexagonal CrN₂
Ken NIWA, Takuro YAMAMOTO, Takuya SASAKI,
 Masashi HASEGAWA
 Nagoya University

C3-12-005 10:45–11:05
Breakdown characteristics of silicon nitrides
Chika MATSUNAGA¹, You ZHOU¹, Dai KUSANO²,
Hideki HYUGA¹, Kiyoshi HIRAO¹
¹National Institute of Advanced Industrial Science and
 Technology, ²Japan Fine Ceramics Co., Ltd.

C3-12-006 11:05–11:25
**High-pressure synthesis and crystal structure of MoC-
 type WN_x**
Takuya SASAKI¹, Takahide IKOMA¹, Kazuki SAGO¹,
Zheng LIU², Ken NIWA¹, Tetsu OHSUNA¹,
Masashi HASEGAWA¹
¹Nagoya University, ²National Institute of Advanced
 Industrial Science and Technology

December 12, 2019

Oral Session 5

Time 14:00–15:45 Room Work-6

Chairperson Ken NIWA

C3-12-I07 ▶ Invited 14:00–14:25
**Room-temperature plastic deformation behavior of ZnS
 crystals under controlled light conditions**
Atsutomo NAKAMURA¹, Yu OSHIMA¹,
Katsuyuki MATSUNAGA^{1,2}
¹Nagoya University, ²Japan Fine Ceramics Center

C3-12-008 14:25–14:45
**Fabrication of Transparent ZnS by Spark-Plasma-
 Sintering (SPS) Technique**
Koji MORITA, Lihong LIU, Tohru S SUZUKI, Byung-Nam KIM
 National Institute for Materials Science (NIMS)

C3-12-009 14:45–15:05
**Evaluation of Microstructure and Interfacial Strength
 of Titanium/Oxide Ceramics Sintered Bonding for
 Biomaterial Application**
Naritoshi AOYAGI, Ryusuke KOIZUMI, Osamu KATAGIRI
 National Institute of Technology, Nagaoka College

C3-12-010 15:05–15:25
**Combustion synthesis of submicron B₄C with induction
 heating assistance**
Anna GUBAREVICH
 Tokyo Institute of Technology

C3-12-011 15:25–15:45
**Control of coarse defects in ceramics formed by dry-
 pressed granules**
Satoshi TANAKA
 Nagaoka University of Technology

December 13, 2019

Oral Session 7

Time 9:30–11:50 Room Port-1

Chairpersons Satoshi KITAOKA, Satoshi TANAKA

C3-13-K01 ▶ Keynote 9:30–10:00
**Nanoscale Dynamic Observations of Grain Boundary
 Fracture, Deformation and Twin Formation in Ceramics**
Yuichi IKUHARA
 University of Tokyo/JFCC

C3-13-I02 ▶ Invited 10:00–10:25
**ULTRA HIGH TEMPERATURE CERAMICS (UHTC) FOR
 HYPERSONIC SPACE VEHICLES: OPPORTUNITIES AND
 CHALLENGES**
Bikramjit BASU
 Indian Institute of Science

C3-13-003 10:25–10:45
**Electric Field-activated Superplastic Deformation in
 Tetragonal Zirconia Polycrystals**
Hidehiro YOSHIDA¹, Yamato SASAKI²,
Takahisa YAMAMOTO³
¹The University of Tokyo, ²Tokyo University of Science,
³Nagoya University

C3-13-I04 ▶ Invited 10:45–11:10
**Extremely Large Room Temperature Strain Tolerant
 Mechanism of Ceramics**
Yutaka KAGAWA
 Tokyo University of Technology

C3-13-005 11:10–11:30
**Evaluation of Delamination Toughness of Atmospheric
 Pressure Plasma Sprayed RTa₃O₅ Thermal Barrier
 Coatings by Simple Shear-loading Method**
Makoto TANAKA¹, Shusui OGAWA¹, Daisaku YOKOE¹,
Satoshi KITAOKA¹, Yuhei OHIDE², Kaito TAKAGI²,
Yoichiro HABU²
¹Japan Fine Ceramics Center, ²TOCALO Co., Ltd.

Symposium A
Symposium B
Symposium C
Symposium D
Symposium E
Symposium F
Symposium G
Symposium H
Symposium I

C3-13-006

11:30–11:50

Criteria of interface crack initiation and propagation in environmental barrier coating with columnar layer under thermal stress

Emi KAWAI¹, Hideki KAKISAWA², Norio YAMAGUCHI¹, Taishi YOKOI¹, Atsushi KUBO³, Satoshi KITAOKA¹, Yoshitaka UMENO³

¹Japan Fine Ceramics Center, ²National Institute for Materials Science, ³The University of Tokyo

December 13, 2019

Oral Session 9

Time 16:30–18:25 Room Port-1

Chairperson Hidehiro YOSHIDA

Preparation

16:30–16:45

C3-13-I07

▶ Invited

16:45–17:05

Mechanical properties of silicon carbide in mesoscale measured by bending test using microcantilever beam specimens

Junichi TATAMI¹, Yumi IMOTO¹, Tsukaho YAHAGI², Takuma TAKAHASHI², Motoyuki IJIMA^{1,2}

¹Yokohama National University, ²Kanagawa Institute of Industrial Science and Technology

C3-13-008

17:05–17:25

Microstructure Control of Al₂O₃-ZrO₂ Composites by Electrostatic Nano-Assembly Technique

Wai Kian TAN, Atsushi YOKOI, Go KAWAMURA, Atsunori MATSUDA, Hiroyuki MUTO
Toyohashi University of Technology

C3-13-009

17:25–17:45

Theoretical Analysis of Densification Kinetics in Final Sintering Stage of Nano-Sized Zirconia

Byungnam KIM¹, Tohru S. SUZUKI¹, Koji MORITA¹, Hidehiro YOSHIDA¹, Ji-Guang LI¹, Hideaki MATSUBARA²

¹National Institute for Materials Science, ²Tohoku University

C3-13-010

17:45–18:05

Observation of internal structure of Al₂O₃ ceramics by optical coherence tomography

Takuma TAKAHASHI¹, Junichi TATAMI^{1,2}, Fumika SAKAMOTO², Hidetaka ITO¹, Isamu TAGUCHI¹, Motoyuki IJIMA^{1,2}

¹Kanagawa Institute of Industrial Science and Technology, ²Yokohama National University

C3-13-011

18:05–18:25

Micromechanics of Sintering: Pinch-off of Pore Channel, Formation and Disappearance of a Closed Pore

Fumihiko WAKAI¹, Gaku OKUMA¹, Norimasa NISHIYAMA¹, Olivier GUILLON²

¹Tokyo Institute of Technology, ²Forschungszentrum Julich

December 12, 2019

Poster Session

Time 16:30–18:00 Room Trade-0

C3-12-P01

Synchrotron X-ray CT imaging of processing-induced defects formed during sintering of alumina

Gaku OKUMA¹, Shuhei WATANABE¹, Kan SHINOBE¹, Norimasa NISHIYAMA¹, Akihisa TAKEUCHI², Kentaro UESUGI², Satoshi TANAKA³, Fumihiko WAKAI¹

¹Tokyo Institute of Technology, ²Japan Synchrotron Radiation Research Institute, JASRI/SPring-8, ³Nagaoka University of Technology

C3-12-P02

Microstructural Design of Composite Materials using Spherical Composite Aggregate Obtained by Electrostatic Nano-assembly Technique

Souta INOUE, Atsushi YOKOI, Wai Kian TAN, Go KAWAMURA, Atsunori MATSUDA, Hiroyuki MUTO

Toyohashi University of Technology

C3-12-P03

Development of thermal conductive PMMA based h-BN composite via electrostatic nano-assembly technique

Atsushi YOKOI, Wai Kian TAN, Go KAWAMURA, Atsunori MATSUDA, Hiroyuki MUTO

Toyohashi University of Technology

C3-12-P04

Phase Transformation and Conducting fluid of Silicon Nitride at High Pressure and Temperature

Yuji KAMISHIMA

Tokyo Institute of Technology

C3-12-P05

Prediction of fracture from various shaped defects by XFEM

Shuhei WATANABE¹, Gaku OKUMA¹, Yosuke SATO², Tomoki SEKIYA¹, Norimasa NISHIYAMA¹, Fumihiko WAKAI¹

¹Laboratory for Materials and Structures Laboratory, Institute of Innovative Research, Tokyo Institute of Technology, ²Mitsubishi Material Corporation Metalworking Solutions Company

C3-12-P06

Fabrication of polycrystalline cotunnite-type zirconia under high pressure and temperature and its mechanical properties.

Palakrit TINNAKORN, Kouki KANATANI, Norimasa NISHIYAMA, Fumihiko WAKAI

Tokyo Institute of Technology

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

C3-12-P07

Fabrication of transparent polycrystalline MgO by combination of spark plasma sintering and high pressure-high temperature synthesis

Masaya ENDO, Gaku OKUMA, Norimasa NISHIYAMA, Fumihiro WAKAI

Tokyo Institute of Technology

C3-12-P08

Synthesis of Single Phase Polycrystals of ω -Titanium and ω -Zirconium under High Pressure and Mechanical Characterization

Takashi SAWAHATA¹, Norimasa NISHIYAMA¹, Makoto ARITA², Fumihiro WAKAI¹, Zenji HORITA²

¹Tokyo Institute of Technology, ²Kyushu University

C3-12-P09

Preparation Of Nitride Phosphor Particle Dispersed Glass Composites

Natsumi TORASE¹, Junichi TATAMI^{1,2}, Motoyuki IJIMA^{1,2}, Takuma TAKAHASHI²

¹Yokohama National University, ²Kanagawa Institute of Industrial Science and Technology

C3-12-P10

Observation of Internal Structure of Al₂O₃ Slurry under Shear by Optical Coherence Tomography

Hiroki TAKABA

Yokohama National University

C3-12-P11

Phase relationship of Si₂N₂O

Kota FUKUCHI

Tokyo Institute of Technology

C3-12-P12

Influence of rare earth oxide as a sintering aid on translucency of aluminum nitride (AlN) ceramics

Hayato AKIMOTO¹, Junichi TATAMI^{1,2}

¹Yokohama National University, ²Kanagawa Institute of Industrial Science and Technology

C3-12-P13

Evolution of anisotropic microstructures in free sintering and constrained sintering of Au sub-micron particles observed by FIB-SEM tomography

Ryo MIYAKI¹, Kan SHINOBE¹, Gaku OKUMA¹, Anna SCIAZKO², Takaaki SHIMURA³, Shotaro HARA⁴, Toshinori OGASHIWA⁵, Naoki SHIKAZONO², Norimasa NISHIYAMA¹, Fumihiro WAKAI¹

¹Tokyo Institute of Technology, ²The University of Tokyo, ³Tokyo University of Agriculture and Technology, ⁴Chiba Institute of Technology, ⁵Tanaka Kikinzoku Kogyo

C3-12-P14

Evaluation of rotation behavior of multilayer graphene coated glass fibers in magnetic field via in situ three-dimensional dynamic observation

Ibuki AIHARA¹, Takuma TAKAHASHI², Junichi TATAMI^{1,2}, Motoyuki IJIMA^{1,2}

¹Yokohama National University, ²Kanagawa Institute of Industrial Science and Technology

C3-12-P15

Crystal Structure and Mechanical Properties of Cr doped Mo₂NiB₂

Junya WATANABE, Toshiki OTA, Satofumi MARUYAMA

Tokyo City University

C3-12-P16

Metal Doping effects on the microstructure and mechanical properties of boron carbide

Toshiki OTA, Ryuichiro KOYAMA, Koga NAKAMURA, Junya WATANABE, Satofumi MARUYAMA

Tokyo City University

C3-12-P17

Mechanical properties of single crystal BaTiO₃ measured using microcantilever beam specimen

Hiroshi YAMAGUCHI¹, Junichi TATAMI^{1,2}, Motoyuki IJIMA^{1,2}

¹Yokohama National University, ²Kanagawa Institute of Industrial Science and Technology

C3-12-P18

In-situ observation of dewaxing process of ceramic powder compacts by optical coherence tomography

Mayu KATO¹, Junichi TATAMI^{1,2}, Motoyuki IJIMA^{1,2}, Takuma TAKAHASHI²

¹Yokohama National University, ²Kanagawa Institute of Industrial Science and Technology

C3-12-P19

Mechanical and Optical Properties of Jadeite/Stishovite and Jadeite/Coelite Ceramic Composites

Eleonora KULIK¹, Alena KRUPP^{1,2}, Astrid HOLZHEID¹, Norimasa NISHIYAMA³, Tetsuo IRIFUNE⁴, Christian RUESSEL⁵, Hiroaki OHFUJI⁴, Youmo ZHOU⁴

¹Institute of Geosciences, Kiel University, Kiel, 24118, Germany, ²Bayerisches Geoinstitut, University of Bayreuth, Bayreuth, 95447, Germany, ³Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology, Yokohama, 226-8503, Japan, ⁴Geodynamics Research Center, Ehime University, Matsuyama, 790-8577, Japan, ⁵Friedrich-Schiller-University Jena, Jena, 07743, Germany

C3-12-P20

Preparation of HfO₂-Al₂O₃ composite films using chemical vapor deposition and their nanostructures

Shogen MATSUMOTO, Akihiko ITO

Yokohama National University

December 12–13, 2019

Symposium C-4

Tough Polymers

[Organizer]

Kohzo ITO (The University of Tokyo)

December 12, 2019

Oral Session 4

Time 9:00–11:30 Room Work-4

Chairpersons Hideyuki OTSUKA, Zhaomin HOU

C4-12-K01 ▶ Keynote 9:00–9:40

Fiber Reinforced Hydrogels With Extra-Ordinarily High Toughness

Jian Ping GONG
Hokkaido University

C4-12-002 9:40–10:00

Crack Propagation of Slide-Ring Gels

Koichi MAYUMI, Chang LIU, Hideaki YOKOYAMA,
Kohzo ITO
The University of Tokyo

C4-12-003 10:00–10:20

Reinforcement of Slide-Ring Hydrogel via Strain-induced Crystallization

Chang LIU¹, Lan JIANG¹, Koichi MAYUMI¹, Takamasa SAKAI²,
Hideaki YOKOYAMA¹, Kohzo ITO¹

¹Department of Advanced Materials Science, Graduate School of Frontier Sciences, The University of Tokyo,

²Department of Bioengineering, Graduate School of Engineering, The University of Tokyo

C4-12-I04 ▶ Invited 10:20–10:50

Velocity Jump in Crack Propagation on Sheet Samples: Nano Scale Glass Transition at a Crack Tip and the Effect of Boundary Condition

Ko OKUMURA
Ochanomizu University

C4-12-005 10:50–11:10

Multi-scale Energy Dissipation Mechanism in Tough and Self-healing Hydrogels

Kunpeng CUI¹, Xueyu LI¹, Xiaobin LIANG², Ken NAKAJIMA²,
Jian Ping GONG¹

¹Hokkaido University, ²Tokyo Institute of Technology

C4-12-006 11:10–11:30

Fatigue Behaviors of Phase Separation Hydrogels: the Effect of Phase Contrast

Xueyu LI¹, Cuipeng CUI², Tao Lin SUN^{1,3},
Takayuki KUROKAWA^{1,3}, Jian Ping GONG^{1,2,3}

¹Soft Matter GI-CoRE, Hokkaido University, ²WPI-ICReDD, Hokkaido University, ³Laboratory of Soft & Wet Matter, Faculty of Advanced Life Science, Hokkaido University

December 12, 2019

Oral Session 5

Time 14:00–16:10 Room Work-4

Chairpersons Yoshinori TAKASHIMA, Jian Ping GONG

C4-12-I07 ▶ Invited 14:00–14:30

Synthesis and Remarkable Self-Healing Properties of Ethylene–Anisylpropylene Copolymers

Zhaomin HOU
RIKEN Center for Sustainable Resource Science

C4-12-008 14:30–14:50

Synthesis of Poly(methyl methacrylate) Based Polyrotaxane via Reversible Addition-Fragmentation Chain Transfer Polymerization

YuCheng WANG¹, Rina MAEDA¹, Gergely KALI²,
Gerhard WENZ², Hideaki YOKOYAMA¹, Kohzo ITO¹
¹Graduate School of Frontier Science, University of Tokyo,
²Organische Makromolekulare Chemie, Universität des Saarlandes

C4-12-I09 ▶ Invited 14:50–15:20

Mechanofunctional Polymers for Self-healing and Stress Visualization Based on Dynamic Covalent Chemistry

Hideyuki OTSUKA, Daisuke AOKI
Tokyo Institute of Technology

C4-12-I10 ▶ Invited 15:20–15:50

Design and Functions of Supramolecular Materials Formed by Reversible and Movable Cross-Linkers

Yoshinori TAKASHIMA
Osaka University

C4-12-011 15:50–16:10

Polybutadienes with Urethane Linkages for Rubber Application

Yasuhiro SHODA^{1,2}, Daisuke AOKI², Katsuhiko TSUNODA¹,
Hideyuki OTSUKA²

¹Bridgestone Corporation, ²Tokyo Institute of Technology

December 12, 2019

Oral Session 6

Time 16:30–18:30 Room Work-4

Chairpersons Kohzo ITO, Hiroshi ITO

C4-12-I12 ▶ Invited 16:30–17:00

Fracture Behaviors of Amorphous Polymer Blends Fabricated by high Shear Kneading Processing

Hiroshi ITO, Akira ISHIGAMI, Kazuki WATANABE,
Yuki KODAMA, Takashi KUROSE, Shotaro NISHITSUJI
Yamagata University

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

C4-12-013 17:00–17:20
The Change of the Density Fluctuations of Amorphous Polymer under Deformation by Using in situ Small Angle X-ray Scattering
SHOTARO NISHITSUJI
 Yamagata University

C4-12-114 ▶ Invited 17:20–17:50
Polyrotaxane Blend Toughened by Movable Crosslinked Structure
Sadayuki KOBAYASHI
 Chemicals Research Laboratories / Japan

C4-12-015 17:50–18:10
Polymer Crystallization under Shear Flow
Go MATSUBA, Kun LI
 Yamagata University

C4-12-016 18:10–18:30
Evaluation of Mechanical Property of Fiber Reinforced Plastics with Extremely Soft Matrix (Soft FRP) from the Perspective of Rehabilitation
Masaki NARISAWA¹, Takahiro KINUGASA¹, Fumihiro INOUE¹, Manabu YAMAGATA², Akiyoshi SAITO³, Junya SUZUKI³, Ryo YONETSU⁴
¹Osaka Prefecture University, ²Kitamura Chemical Co. Ltd., ³Kawamura Gishi Co. Ltd., ⁴Kanagawa University of Human Services

December 13, 2019

Oral Session 7

Time 9:00–11:40 **Room** Work-4

Chairpersons Keiji TANAKA, Taiki HOSHINO

C4-13-101 ▶ Invited 9:00–9:40
Synchrotron Radiation X-ray Scattering Study of Multiphase Polymers under Mechanical Deformation
Atsushi TAKAHARA, Ken KOJIO, Nattanee DECHNARONG, Chao-Hung CHENG
 Kyushu University

C4-13-102 ▶ Invited 9:40–10:10
Building a New Range of Synchrotron Radiation Application to the Research of Tough Polymers
Taiki HOSHINO¹, Yusuke TAMENORI², Shuji GOTO², Masaki TAKATA³
¹RIKEN SPring-8 Center, ²JASRI, ³Tohoku University

C4-13-003 10:10–10:30
Structural Analysis in Nanocomposite Elastomer with Block Copolymer-Grafted Silica Particles by Synchrotron Radiation X-ray Scattering and Spectroscopy under Various Mechanical Deformation
Chao-Hung CHENG¹, Shuhei NOZAKI¹, Shiori MASUDA¹, Nattanee DECHNARONG¹, Kiyu UNO¹, Kazutaka KAMITANI², Ken KOJIO^{1,2,3}, Atsushi TAKAHARA^{1,2,3}
¹Graduate School of Engineering, Kyushu University, ²IMCE, Kyushu University, ³WPI-I2CNER, Kyushu University

C4-13-104 ▶ Invited 10:30–11:00
Innovative Tough Rubber Compound for Environmental Friendly Tire
Katsuhiko TSUNODA
 Bridgestone Corporation

C4-13-005 11:00–11:20
Aggregation States and Thermal Molecular Motion of Fluororubber Chains Adsorbed onto Model Carbon Interfaces
Daiki SAITO¹, Kazuki SASAHARA², Yoshihisa TAKEYAMA³, Mitsugi UEJIMA³, Daisuke KAWAGUCHI², Satoru YAMAMOTO², Keiji TANAKA^{1,2}
¹Department of Automotive Science, Kyushu University, ²Department of Applied Chemistry, Kyushu University, ³Zeon Corporation

C4-13-006 11:20–11:40
Change in Molecular Aggregation State and Rupture Mechanism of Poly(methyl methacrylate) and Polycarbonate Films during Bulge Testing
Ken KOJIO^{1,2,3}, Aya FUJIMOTO¹, Tomoko KAJIWARA¹, Chigusa NAGANO², Chao-Hung CHENG², Shuhei NOZAKI², Shiori MASUDA², Nattanee DECHNARONG², Kazutaka KAMITANI¹, Atsushi TAKAHARA^{1,2,3}
¹Institute for Materials Chemistry and Engineering, Kyushu University, ²Graduate School of Engineering, Kyushu University, ³International Institute for Carbon-Neutral Energy Research, Kyushu University

December 13, 2019

Oral Session 9

Time 16:30–18:30 **Room** Miel-5

Chairpersons Susumu OKAZAKI, Atsushi TAKAHARA

C4-13-107 ▶ Invited 16:30–17:00
Showered Dynamics of Polymer Dynamics at Inorganic-filler Interface
Keiji TANAKA¹, Hung K. NGUYEN¹, Manabu INUTSUKA², Daisuke KAWAGUCHI¹
¹Kyushu University, ²Kanagawa University

C4-13-008 17:00–17:20
Characterization of Tough Polymer Interfaces by Interface-Sensitive Spectroscopy
Daisuke KAWAGUCHI¹, Shin SUGIMOTO², Satoru YAMAMOTO¹, Keiji TANAKA^{1,2}
¹Department of Applied Chemistry, Kyushu University, ²Department of Automotive Science, Kyushu University

C4-13-109 ▶ Invited 17:20–17:50
All-Atomistic Molecular Dynamics Study of Impact Fracture of Glassy Polymers
Susumu OKAZAKI, Kazushi FUJIMOTO, Zhiye TANG
 Nagoya University

C4-13-010

17:50–18:10

Network Heterogeneity and Fracture Behavior in Epoxy Resin

Satoru YAMAMOTO, Mika AOKI, Atsuomi SHUNDO,
Keiji TANAKA
Kyushu University

C4-13-011

18:10–18:30

Stress Relaxation Mechanism of Slide-Ring gels: A Coarse-Grained Molecular Dynamics Simulation Study.

Yusuke YASUDA¹, Koichi MAYUMI¹, Masatoshi TODA²,
Hideaki YOKOYAMA¹, Hiroshi MORITA², Kohzo ITO¹

¹Department of Advanced Materials Science, School of Frontier Sciences, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8561, Japan., ²National Institute of Advanced Industrial Science and Technology (AIST), 1-1-1, Umezono, Tsukuba, Ibaraki 305-8568, Japan.

December 13, 2019

Poster Session

Time 19:00–20:30 Room Trade-0

C4-13-P01

One-pot synthesis of polyrotaxane with different host coverage and its slide-ring materials

Lan JIANG, Chang LIU, Koichi MAYUMI, Hideaki YOKOYAMA,
Kohzo ITO
The University of Tokyo

C4-13-P02

The Synthesis of the Polycyclooctadiene-based Polyrotaxane with Thermally Resistant

Randi ZHANG¹, Lan JIANG¹, Hideaki YOKOYAMA¹,
Wen-hua SUN², Kohzo ITO¹

¹University of Tokyo, ²University of Chinese Academy of Sciences

C4-13-P03

Photoregulation of the Heat Resistance in Network Polymers with Diarylethene-conjugated Diels–Alder Cross-links

Jumpei KIDA, Daisuke AOKI, Hideyuki OTSUKA
Tokyo Institute of Technology

C4-13-P04

Preparation of Materials with Supramolecular Cross-linking and Their Physical Properties

Ryohei IKURA¹, Junsu PARK¹, Motofumi OSAKI¹,
Hiroyasu YAMAGUCHI¹, Akira HARADA²,
Yoshinori TAKASHIMA^{1,3}

¹Department of Macromolecular Science, Graduate School of Science, Osaka University, ²The Institute of Scientific and Industrial Research, Osaka University, ³Institute for Advanced Co-Creation Studies, Osaka University

C4-13-P05

Synthesis of Reactive Polymer/silica Nanocomposites with Dynamic Covalent Bonds at the Filler-matrix Interface

Shimon KATAOKA
Department of Chemical Science and Engineering, Tokyo
Institute of Technology

C4-13-P06

Modification of Amine-Cured Epoxy Resins by Boronic Acids

Yumiko ITO, Daisuke AOKI, Hideyuki OTSUKA
Tokyo Institute of Technology

C4-13-P07

Tough and Functional Supramolecular Materials from Polymer Mixtures with Host-guest Interaction between Cyclodextrin and Adamantane

Junsu PARK¹, Motofumi OSAKI¹, Yoshinori TAKASHIMA^{1,2},
Akira HARADA³, Hiroyasu YAMAGUCHI¹

¹Graduate School of Science, Osaka University, ²IACS, Osaka University, ³ISIR, Osaka University

C4-13-P08

Toughening Polymer Networks via Freezing-Induced Radical Generation Based on Mechanocleavable Fluorescent Dynamic Covalent Bonds

Sota KATO, Daisuke AOKI, Hideyuki OTSUKA
Tokyo Institute of Technology

C4-13-P09

Facile Visualization of Molecular-level Slide-ring Effect via Mechanochromic Chemistry

Yi LU, Daisuke AOKI, Hideyuki OTSUKA, Toshikazu TAKATA
Tokyo Institute of Technology

C4-13-P10

Force-induced Cross-linking Reaction in a Radical-Type Mechanochromic Polyurethane with Polymerizable Side Chains

Kota SESHIMO, Hio SAKAI, Daisuke AOKI, Hideyuki OTSUKA
Tokyo Institute of Technology

C4-13-P11

Supramolecular Ionic Liquid Elastomer based on Host-Guest Interactions

Garry SINAWANG¹, Yuichiro KOBAYASHI¹,
Yoshinori TAKASHIMA^{1,2}, Akira HARADA³,
Hiroyasu YAMAGUCHI¹

¹Graduate School of Science, Osaka University, ²Institute for Advanced Co-Creation Studies, Osaka University, ³The Institute of Scientific and Industrial Research, Osaka University

C4-13-P12

Designed Polymer Network Structure Using 4-arm and 2-arm PEGs in Ionic Liquid-Based Electrolytes for Lithium-Ion Batteries

Asumi ISHIKAWA, Kenta FUJII
Yamaguchi University

C4-13-P13

Chromonic Aggregates-Incorporated Tough Hydrogels

Khoa LE

Tokyo University of Science

C4-13-P14

Relationship between the Dissociation Energy of Reversible Cross-links and Mechanical Properties of Supramolecular Hydrogels with Inclusion Complexes.

Subaru KONISHI¹, Yoshinori TAKASHIMA^{1,2}, Akira HARADA³, Hiroyasu YAMAGUCHI¹¹Graduate School of Science, Osaka University, ²Institute for Advanced Co-Creation Studies, Osaka University, ³Institute of Scientific and Industrial Research, Osaka University

C4-13-P15

Evaluation of Toughness and Failure Mode of PA6/mSEBS/PS Ternary Blends with and Oil Extended Viscoelastic Controlled Interface

Akira ISHIGAMI

Yamagata University

C4-13-P16

Elastomeric Nanocomposites Composed of Silica Nanoparticles with End-Functionalized Rubbery Polymer Brush

Kiyu UNO¹, Atsushi TAKAHARA^{1,2,3}, Yuji HIGAKI⁴, Ken KOJIO^{1,2,3}, Hitoshi SHIMAMOTO¹, Kazutaka KAMITANI², Masaru MUKAI², Chao-Hung CHENG¹¹graduate school of engineering, Kyushu University, ²IMCE, ³WPI-I2CNER, ⁴Faculty of Science technology, Oita University

C4-13-P17

Structural Analysis of Japanese Sweets -Warabi-mochi-

Akane NAGASAKI, Go MATSUBA

Yamagata University

C4-13-P18

Precise Structural Analysis Bi-axially Stretched Films

Keisuke SOTOYAMA, Go MATSUBA

Yamagata University

C4-13-P19

In Situ Small-Angle X-Ray Scattering Investigation on Mesoscopic Deformation of Thermoplastic Elastomer under Cyclic ElongationsNattanee DECHNARONG¹, Kazutaka KAMITANI², Chao-Hung CHENG¹, Shiori MASUDA¹, Shuhei NOZAKI¹, Chigusa NAGANO¹, Ken KOJIO^{1,2,3}, Atsushi TAKAHARA^{1,2,3}¹Graduate School of Engineering, Kyushu University, ²Institute for Materials Chemistry and Engineering, Kyushu University, ³International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University

C4-13-P20

Quasi-two-dimensional coalescence of liquid in another liquid

Yukina Margaret KOGA

Ochanomizu University

C4-13-P21

Molecular Dynamics Study of Compressive Fracture of Glassy Polymers

Hiroaki ISHIKAWA, Kazushi FUJIMOTO, Zhiye TANG, Susumu OKAZAKI

Graduate School of Engineering, Nagoya University

C4-13-P22

All-atom Molecular Dynamics Study of Impact Fracture of Glassy Polymers: Molecular Mechanism of Brittleness and Ductility

Zhiye TANG, Kazushi FUJIMOTO, Wataru SHINODA, Susumu OKAZAKI

Nagoya University

C4-13-P23

Molecular Study of Impact Fracture of Amorphous Polymer I: Brittle and Ductile

Kazushi FUJIMOTO

Nagoya University

Cluster D

Advanced Electronic Materials

Symposium

- D-1** 2D Layered Materials
- D-2** Novel Concepts of Electronic Materials Inspired from Complementary and Competing Fields
- D-3** Science and Technology of Superconductivity
- D-4** **5th E&J BLS** Wide-bandgap and 2-dimensional Materials

December 11–13, 2019

Symposium D-1

2D Layered Materials

[Organizers]

Susumu SAITO (Tokyo Institute of Technology)
Yoshihiro IWASA (University of Tokyo)
Yuanbo ZHANG (Fudan University)

[Sponsor]



Nanocarbon research committee,
Foundation Advanced Technology Institute

December 11, 2019

Oral Session 1

Time 9:00–11:30 Room Work-4

Chairperson Susumu SAITO

Opening

9:00–9:30

D1-11-K01 ▶ Keynote 9:30–10:15

Exploring 2D Materials: From Nanopores to Ordered Alloys to e-Beam Induced Circuitry

Alex ZETTL

University of California at Berkeley

D1-11-I02 ▶ Invited 10:15–10:45

Optical and vibrational EELS from low-dimensional materials

Kazutomo SUENAGA

AIST

D1-11-003 10:45–11:00

Change in the photo response by Adsorption of Phthalocyanine Complex Molecules on MoS₂-FET

Hiroki WAIZUMI¹, Tsuyoshi TAKAOKA², Kazuki WASHIDA¹, Md Iftekharul ALAM¹, Muhammed Shamim AI MAMUN¹, Tat Trung NGUYEN¹, Tadahiro KOMEDA²

¹Faculty of Science, Tohoku University, ²IMRAM, Tohoku University

D1-11-004 11:00–11:15

Molecular adsorption and electronic properties of doped graphene for sensing applications

Yoshitaka FUJIMOTO¹, Susumu SAITO^{1,2,3}

¹Department of Physics, Tokyo Institute of Technology, ²Advanced Research Center for Quantum Physics and Nanoscience, Tokyo Institute of Technology, ³Materials Research Center for Element Strategy, Tokyo Institute of Technology

D1-11-005 11:15–11:30

Effect of The Adsorption of TCNQ And F4-TCNQ On MoS₂-based FET

Tsuyoshi TAKAOKA, Tat Trung NGUYEN, Md Iftekharul ALAM, Kazuki WASHIDA, Hiroki WAIZUMI, Muhammed Shamim ALMAMUN, Tadahiro KOMEDA
Tohoku University

December 11, 2019

Oral Session 2

Time 14:00–16:00 Room Work-4

Chairperson Yoshihiro IWASA

D1-11-K06 ▶ Keynote 14:00–14:45

Quantum transport and robotic fabrication of van der Waals junctions of graphene and 2D materials

Tomoki MACHIDA

Institute of Industrial Science, University of Tokyo

D1-11-I07 ▶ Invited 14:45–15:15

Charge transfer dynamics at two-dimensional material/liquid electrolyte interfaces

Chun-Wei CHEN

National Taiwan University

D1-11-008 15:15–15:30

Honeycomb lattice based electrides: Electronic structures and catalytic applications towards selective hydrogenation

Yangfan LU¹, TIAN NAN YE¹, Jian LI¹, Takuya NAKAO², Yoshitake TODA¹, Shigenori UDEA³, Tomofumi TADA¹, Koji HORIBA⁴, Hiroshi KUMIGASHIRA⁴, Masaaki KITANO¹, Hideo HOSONO¹

¹Materials Research Center for Element Strategy, Tokyo Institute of Technology, ²Laboratory for Materials and Structures, Tokyo Institute of Technology, ³Synchrotron X-ray Station at SPring-8, National Institute for Material Science (NIMS), ⁴Photon Factory and Condensed Matter Research Center, Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK)

D1-11-009 15:30–15:45

Concerted Nanoporosity of H₂O-adsorbed GOs, Evidenced by in-situ X-ray Diffractions

Ryusuke FUTAMURA¹, Taku IYAMA^{1,2}, Takahiro UEDA^{3,4}, Katsumi KANEKO²

¹Department of Chemistry, Shinshu University, ²Research Initiative for Supra-Materials, Shinshu University, ³The Museum of Osaka University, ⁴Department of Chemistry, Graduate School of Science, Osaka University

D1-11-010 15:45–16:00

Novel friction induced crystal growth of 2D layered MoS₂ on semiconductor surfaces

Tadao TANABE, Takafumi ITO, Junya OSAKI, Chao TANG, Yohei SATO, Yutaka OYAMA

Tohoku University

December 11, 2019

Oral Session 3**Time** 16:30–18:30 **Room** Work-4

Chairperson Hiroki AGO

D1-11-I11 ▶ Invited 16:30–17:00

Nanophotonics with Hexagonal Boron Nitride

Igor AHARONOVICH
UTS**D1-11-I12** ▶ Invited 17:00–17:30

Optical Physics in Two-dimensional Layered Materials and its Hetero-structures

Kazunari MATSUDA
Kyoto University**D1-11-013** 17:30–17:45Large Photoluminescence Enhancement of Monolayer MoS₂ by a Molecular Treatment with the Aid of UV IrradiationYuki YAMADA¹, Yuki AOKI¹, Akito HUKUI¹, Yuji MATSUSHITA¹, Takeshi YOSHIMURA¹, Atsushi ASHIDA¹, Norifumi FUJIMURA¹, Keisuke SHINOKITA³, Kazunari MATSUDA³, Daisuke KIRIYA^{1,2}
¹Osaka Prefecture University, ²JST PRESTO, ³Institute of Advanced Energy, Kyoto University**D1-11-014** 17:45–18:00

Photodetectors based on bilayer graphene heterostructure FETs

Teerayut UWANNO^{1,2}, Takashi TANIGUCHI³, Kenji WATANABE³, Kosuke NAGASHIO¹¹University of Tokyo, ²King Mongkut's institute of technology Ladkrabang, ³National institute of materials science**D1-11-015** 18:00–18:15

Anomalous Hall effect in atomically-thin chromium telluride thin film grown by molecular-beam epitaxy

Yue WANG¹, Masaki NAKANO^{1,2}, Satoshi YOSHIDA¹, Hideki MATSUOKA¹, Kyoko ISHIZAKA^{1,2}, Yoshihiro IWASA^{1,2}
¹Dept. of Appl. phys, Univ. of Tokyo, ²RIKEN CEMS

Post-deadline Invited presentation
by Kaya Kobayashi
18:15–18:30

December 12, 2019

Oral Session 4**Time** 9:00–11:30 **Room** Mont-3

Chairperson Mikito KOSHINO

Symposium breakfast meeting 1

9:00–9:30

D1-12-K01 ▶ Keynote 9:30–10:15

Roles of Interlayer Interactions in Stacked 2D Crystals

Young-Woo SON
Korea Institute for Advanced Study**D1-12-I02** ▶ Invited 10:15–10:45

Continue the transistor scaling with 2D materials: Challenges and Perspectives

Lain-Jong LI
TSMC**D1-12-003** 10:45–11:00

Topological Edge States of Monolayer Black Phosphorene

Masaru HITOMI, Mikito KOSHINO
Osaka University**D1-12-004** 11:00–11:15Room-Temperature Valley-Polarized Light-Emitting Devices *via* Strained Monolayer SemiconductorsJiang PU¹, Hirofumi MATSUOKA¹, Yu KOBAYASHI², Yasumitsu MIYATA², Taishi TAKENOBU¹¹Nagoya University, ²Tokyo Metropolitan University**D1-12-005** 11:15–11:30

Geometries and Electronic Properties of Transition Metal Dichalcogenide Nanotubes

Shuntaro OSHIMA¹, Masayuki TOYODA¹, Susumu SAITO^{1,2,3}
¹Department of Physics, Tokyo Institute of Technology, Meguro, Tokyo, 152-8551, Japan, ²Advanced Research Center for Quantum Physics and Nanoscience, Tokyo Institute of Technology, Meguro, Tokyo 152-8551, Japan, ³Materials Research Center for Element Strategy, Tokyo Institute of Technology, Yokohama, Kanagawa 226-8503, Japan

December 12, 2019

Oral Session 6**Time** 16:30–18:30 **Room** Mont-3

Chairperson Kosuke NAGASHIO

D1-12-I06 ▶ Invited 16:30–17:00

Silicene and Beyond: Experimental Realization of Group IV 2D Materials

Yukiko YAMADA-TAKAMURA
Japan Advanced Institute of Science and Technology

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

D1-12-I07 ▶ Invited 17:00–17:30
Geometric and Electronic Structures of Hybridstructure of 2D Materials
Susumu OKADA
 University of Tsukuba

D1-12-008 17:30–17:45
Crossover between Orbital limit and Pauli-paramagnetic limit in ultra-thin NbSe₂
Hideki MATSUOKA¹, Masaki NAKANO^{1,2},
Yoshimitsu KOHAMA³, Yue WANG¹, Yuta KASHIWABARA¹,
Satoshi YOSHIDA¹, Kazuki MATSUI³, Takashi SHITAOKOSHI¹,
Takumi OUCHI⁴, Kyoko ISHIZAKA^{1,2}, Tsutomu NOJIMA⁴,
Masashi KAWASAKI^{1,2}, Yoshihiro IWASA^{1,2}
¹The University of Tokyo, ²RIKEN Center for Emergent Matter Science (CEMS), ³Institute for Solid State Physics, University of Tokyo, ⁴Institute for Materials Research, Tohoku University

D1-12-009 17:45–18:00
Ambipolar transistor action of germanane electric double layer transistor
Yumiko KATAYAMA, Ryoto YAMAUCHI, Yusuke YASUTAKE,
Susumu FUKATSU, Kazunori UENO
 The University of Tokyo

D1-12-010 18:00–18:15
Transparency and Two-dimensional Hole Superconductivity in Li_{1-x}NbO₂
Takuto SOMA¹, Kohei YOSHIMATSU¹, Akira OHTOMO^{1,2}
¹Tokyo Institute of Technology, ²Materials Research Center for Element Strategy (MCES)

D1-12-011 18:15–18:30
Thickness-dependent Optical Bandgap and Electrical Transport Properties in Layered InSe Thin Films Grown by Pulsed-laser Deposition
Dingheng ZHENG, Junichi SHIOGAI, Kohei FUJIWARA,
Atsushi TSUKAZAKI
 Institute for Materials Research, Tohoku University, Sendai, 980-8577, Japan

December 13, 2019

Oral Session 7

Time 9:00–11:30 Room Mont-3

Chairperson Tomoki MACHIDA

[Symposium breakfast meeting 2
 9:00–9:30]

D1-13-K01 ▶ Keynote 9:30–10:15
Ruoff Group Carbon Research
Rodney RUOFF
 UNIST

D1-13-I02 ▶ Invited 10:15–10:45
Moiré phonons in the twisted bilayer graphene
Mikito KOSHINO¹, Young Woo SON²
¹Osaka University, ²Korea Institute for Advanced Study

D1-13-003 10:45–11:00
Nonreciprocal transport and anomalous photovoltaic effect in van der Waals nanomaterials
Toshiya IDEUE¹, Yoshihiro IWASA^{1,2}
¹The University of Tokyo, ²RIKEN CEMS

D1-13-004 11:00–11:15
General theory on the electronic states in layered materials with commensurate interlayer shift
Ryosuke AKASHI
 The University of Tokyo

D1-13-005 11:15–11:30
Quantum and classical ratchet motions of vortices in a 2D trigonal superconductor MoS₂
Yuki ITAHASHI¹, Yu SAITO¹, Toshiya IDEUE¹,
Tsutomu NOJIMA², Yoshihiro IWASA^{1,3}
¹Department of applied physics, The University of Tokyo, ²Institute for Materials Research, Tohoku University, ³RIKEN Center for Emergent Matter Science (CEMS)

December 13, 2019

Oral Session 8

Time 14:00–16:00 Room Mont-3

Chairperson Susumu OKADA

D1-13-I06 ▶ Invited 14:00–14:30
High-throughput synthesis of graphene by plasma CVD
Masataka HASEGAWA, Ryuichi KATO, Wararu MIZUTANI,
Masatou ISHIHARA, Takatoshi YAMADA, Yuki OKIGAWA
 AIST

D1-13-I07 ▶ Invited 14:30–15:00
Controlled CVD Growth of High-Quality 2D Layered Materials for Electronic and Photonic Applications
Hiroki AGO
 Kyushu University

D1-13-008 15:00–15:15
Electronic properties of graphene/C-doped h-BN heterostructures
Taishi HAGA¹, Yoshitaka FUJIMOTO¹, Susumu SAITO^{1,2,3}
¹Department of Physics, Tokyo Institute of Technology, ²Advanced Research Center for Quantum Physics and Nanoscience, Tokyo Institute of Technology, ³Materials Research Center for Element Strategy, Tokyo Institute of Technology

D1-13-009

15:15–15:30

Direct observation of electron capture & emission processes by the time domain charge pumping measurement of MoS₂ FET

Kosuke NAGASHIO, Koki TANIGUCHI, Nan FANG
The University of Tokyo

D1-13-010

Withdrawal

D1-13-011

15:30–15:45

THz optical and electrical properties, and the interlayer mechanical properties of InSe crystals grown from the liquid phase

Chao TANG, Yohei SATO, Katsuya WATANABE,
Junya OSAKI, Tadao TANABE, Yutaka OYAMA
Tohoku University

Closing
15:45–16:00

December 11, 2019

Poster Session

Time 19:00–20:30 Room Trade-0

D1-11-P01

Trion-based High-speed Carbon Nanotube Films
Electroluminescence Emitters

Hidegori TAKAHASHI¹, Yuji SUZUKI¹, Norito YOSHIDA¹,
Kenta NAKAGAWA², Hideyuki MAKI¹
¹Keio University, ²KISTEC

D1-11-P02

Electronic Correlation in the Two-Dimensional Electride
Y₂C

Masatoshi HIRAISHI¹, Kenji KOJIMA^{1,2}, Ichihiro YAMAUCHI¹,
Hirotaka OKABE¹, Soshi TAKESHITA¹, Akihiro KODA^{1,2},
Ryosuke KADONO^{1,2}, Xiao ZHANG³, Satoru MATSUIISHI⁴,
Hideo HOSONO^{3,4}, Kazuto HIRATA⁵, Shigeki OTANI⁵,
Naoki OHASHI⁵
¹KEK IMSS, ²SOKENDAI, ³MSL, ⁴MCES, ⁵NIMS

D1-11-P03

Polymorphs of Transition Metal Dichalcogenide and the
superconductivity modulated by the structures

Sana SASAKURA¹, Jun AKIMITSU², Kaya KOBAYASHI^{1,2}
¹Graduate school of Natural Science and Technology,
Okayama University, ²RIIS, Okayama University

D1-11-P04

Electronic Structure of Periodically Modified Graphene

Tomoya ITO¹, Susumu SAITO^{1,2,3}

¹Department of Physics, Tokyo Institute of Technology,
²Advanced Research Center for Quantum Physics and
Nanoscience, Tokyo Institute of Technology, ³Materials
Research Center for Element Strategy, Tokyo Institute of
Technology

D1-11-P05

Growth and transport properties of monolayer MoSe₂/
WSe₂ in-plane heterostructures

Hiroshi SHIMIZU
Tokyo Metropolitan University

D1-11-P06

Optical Absorption of The Circularly-Polarized Light
Irradiation in Triptycene Molecular Membrane

Masashi AKITA
Department of Nanotechnology for Sustainable Energy,
School of Science and Technology Kwansei Gakuin
University

D1-11-P07

Co-Intercalation of Metal Chlorides in Large-Area Bilayer
Graphene

Amane MOTOYAMA¹, Kenji KAWAHARA²,
Rika MATSUMOTO³, Hiroki AGO^{1,2}

¹Kyushu University, ²Global Innovation Center, ³Tokyo
Polytechnic University

D1-11-P08

Influence of Pore Density of Porous Epitaxial Graphene
on Aniline Polymerization

Ryuichi HIRAI, Akihiro HASHIMOTO
University of Fukui

D1-11-P09

Topological Pump Induced by Dynamics of Moiré Pattern

Manato FUJIMOTO, Mikito KOSHINO
Osaka University

D1-11-P10

Doping Magnetic Impurity Into Valley Materials by
Molecular Beam Epitaxy

Yuki MAJIMA¹, Yuta KASHIWABARA¹, Hideki MATSUOKA¹,
Masaki NAKANO^{1,2}, Yoshihiro IWASA^{1,2}

¹University of Tokyo, ²RIKEN Center for Emergent Matter
Science (CEMS)

D1-11-P11

Low Temperature Liquid Phase Growth of 2D Layered
Semiconductor GaSe by Flux Method and Evaluation of
Nonlinear Optical Characteristics

Katsuya WATANABE, Yohei SATO, Chao TANG, Junya OSAKI,
Tadao TANABE, Chen MINGXI, Yutaka OYAMA
University of Tohoku

D1-11-P12

Electric Double Layer Transistors of CVD-grown monolayers InSe and InS

Jiang PU¹, Han-Ching CHANG², Chien-Liang TU²,
Kuang-I LIN³, Chien-Nan HSIAO⁴, Chang-Hsiao CHEN^{2,5},
Taishi TAKENOBU¹

¹Nagoya University, ²Feng Chia University, ³National Cheng Kung University, ⁴National Applied Research Laboratory, ⁵National Sun Yat-sen University

D1-11-P13

Electronic properties in hBN-graphene-hBN trilayer systems

Hiroki OKA

Department of Physics, Osaka University

D1-11-P14

Development of an Electron Doping Method Using Specific Interaction between Amide Molecule and MoS₂

Akito FUKUJ¹, Yuh HIJIKATA², Jenny PIRILLO²,
Takeshi YOSHIMURA¹, Atsushi ASHIDA¹,
Norifumi FUJIMURA¹, Daisuke KIRIYA^{1,3}

¹Osaka Prefecture University, ²Hokkaido University, ³JST PRESTO

D1-11-P15

Misfit chalcogenide superconductors: (BiSe)_{1+n}(NbSe₂)_m

Masaharu SHIRATA¹, Jun AKIMITSU², Kaya KOBAYASHI^{1,2}

¹Department of Physics, Okayama University, ²RiiS, Okayama University

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 11–12, 2019

Symposium D-2Novel Concepts of Electronic Materials Inspired
from Complementary and Competing Fields

[Organizer]

Toshio KAMIYA (Tokyo Institute of Technology)

December 12, 2019

Oral Session 4

Time 9:00–11:30 Room Work-7

Chairperson Toshio KAMIYA

break
9:00–9:30

D2-12-I01 ▶ Invited 9:30–10:00

**Materials Design of Functional Semiconductors
with Light Emission and Carrier Dopabilities: Ternary
Perovskite Sulfides AEHfS₃ (AE=Sr & Ba)**Kota HANZAWA¹, Soshi IIMURA², Hidenori HIRAMATSU^{1,2},
Hideo HOSONO²¹Laboratory for Materials and Structures, Tokyo Institute
of Technology, ²Materials Research Center for Element
Strategy, Tokyo Institute of Technology

D2-12-002 10:00–10:15

**Light emitting diodes on glass using amorphous oxide
semiconductor thin-film phosphors, rare-earth doped
a-Ga-O**Naoto WATANABE¹, Keisuke IDE^{1,2}, Takayoshi KATASE^{1,3},
Junghwan KIM², Shigenori UEDA^{4,5}, Koji HORIBA⁶,
Hiroshi KUMIGASHIRA⁶, Hidenori HIRAMATSU^{1,2},
Hideo HOSONO^{1,2}, Toshio KAMIYA^{1,2}¹Laboratory for Materials and Structures, Tokyo Institute
of Technology, ²Materials Research Center for Element
Strategy, Tokyo Institute of Technology, ³PRESTO, Japan
Science and Technology Agency, ⁴National Institute for
Materials Science, ⁵Synchrotron X-ray Station at SPring-8,
⁶High Energy Accelerator Research Organization

D2-12-003 10:15–10:30

**Fabrication of electrochromic transistor on flexible
substrate**Takaki ONOZATO¹, Hai Jun CHO^{1,2}, Hiromichi OHTA^{1,2}¹Graduate School of Information Science and Technology,
Hokkaido University, ²Research Institute for Electronic
Science, Hokkaido University

D2-12-004 10:30–10:45

**Enhanced thermoelectric power-factors by strain control
in strongly correlated lanthanum titanate**Takayoshi KATASE, Keisuke IDE, Hidenori HIRAMATSU,
Hideo HOSONO, Toshio KAMIYA

Tokyo Institute of Technology

D2-12-005 10:45–11:00

**Density Functional Study on Defects and Doping for
Layered Ternary Nitride, SrTiN₂**XINYI HE¹, Zewen XIAO^{2,3}, Takayoshi KATASE^{1,4},
Keisuke IDE¹, Hideo HOSONO^{1,2}, Toshio KAMIYA^{1,2}¹MSL, Tokyo Tech, Yokohama, Japan, ²MCES, Tokyo
Tech, Yokohama, Japan, ³Wuhan National Laboratory
for Optoelectronics, Huazhong University of Science and
Technology, China, ⁴PRESTO, JST, Tokyo, Japan

D2-12-006 11:00–11:15

**Anisotropic Exponential Optical Absorption Edge in PbS
Quantum Dots on the (001), (110), and (111) Surfaces
of Single Crystal Rutile-TiO₂: Comparative Study on
Photoacoustic and Absorbance Spectra**Taro TOYODA¹, Qing SHEN¹, Keita KAMIYAMA²,
Shuzi HAYASE³¹The University of Electro-Communications, ²bunkoukeiki
Co., Ltd., ³Kyushu Institute of Technology

D2-12-007 11:15–11:30

**Room-Temperature Control of Non-reciprocal Microwave
Response in Multiferroic Y-type Hexaferrite**Sakyo HIROSE¹, Yoichi NII², Tsuyoshi KIMURA³,
Yoshinori ONOSE²¹Murata Manufacturing Co., Ltd., ²Institute for Materials
Research, Tohoku University, ³Department of Advanced
Materials Science, University of Tokyo

December 12, 2019

Oral Session 6

Time 16:30–18:30 Room Work-7

Chairperson Toshio KAMIYA

D2-12-I08 ▶ Invited 16:30–17:00

**Shift current: a new perspective on ferroelectric
photovoltaics**Masao NAKAMURA¹¹RIKEN Center for Emergent Matter Science (CEMS),
²PRESTO Japan Science and Technology Agency (JST)

D2-12-I09 ▶ Invited 17:00–17:30

**Novel Applications of ferroelectric and semiconducting
perovskite oxide films**Norifumi FUJIMURA
Osaka Prefecture Univ.

D2-12-I10 ▶ Invited 17:30–18:00

**Phase stability and property control of ferroelectric HfO₂
films**Hiroshi FUNAKUBO, Takanori MIMURA, Takao SHIMIZU
Tokyo Institute of Technology

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

D2-12-011

18:00–18:15

Dielectric properties of ReO₃-type oxyfluorides prepared by hydrothermal synthesis

 Masanori KODERA¹, Ayako TAGUCHI², Takao SHIMIZU³, Hiroki MORIWAKE², Hiroshi FUNAKUBO^{1,3}
¹Material Research Center for Element Strategy, Tokyo Institute of Technology, ²Japan Fine Ceramics Center, ³School of Materials and Chemical Technology, Tokyo Institute of Technology

D2-12-012

18:15–18:30

Single Crystal Growth and Intrinsic Electron Mobility of Cubic SrGeO₃

 Christian A. NIEDERMEIER¹, Yu KUMAGAI², Keisuke IDE^{1,2}, Takayoshi KATASE^{1,2}, Fumiyasu OBA^{1,2,3}, Hideo HOSONO^{1,2}, Toshio KAMIYA^{1,2}
¹Laboratory for Materials and Structures, Tokyo Institute of Technology, Yokohama, 226-8503, Japan, ²Materials Research Center for Element Strategy, Tokyo Institute of Technology, Yokohama, 226-8503, Japan, ³Center for Materials Research by Information Integration, National Institute for Materials Science, Tsukuba, Ibaraki 305-0047, Japan

December 11, 2019

Poster Session
Time 19:00–20:30 **Room** Trade-0

D2-11-P01

Structural phase transition and opto-electronic properties of oxide semiconductor solid solution, (Ba,Sr)(Sn,Ti)O₃

 Yutaro KOBAYASHI¹, Keisuke IDE¹, Takayoshi KATASE^{1,2}, Hidenori HIRAMATSU^{1,3}, Hideo HOSONO^{1,3}, Toshio KAMIYA^{1,3}
¹Laboratory for Materials and Structures, Tokyo Institute of Technology, ²PRESTO, Japan Science and Technology Agency, ³Materials Research Center for Element Strategy, Tokyo Institute of Technology

D2-11-P02

Investigation of Anionic Electron-Induced Magnetism in a Two Dimensional Electride Y₂C by Inelastic Neutron Scattering

 Hiromu TAMATSUKURI¹, Youichi MURAKAMI¹, Hajime SAGAYAMA¹, Satoru MATSUSHI², Yasuhito WASHIO², Masato MATSUURA³, Yukinobu KAWAKITA⁴, Hideo HOSONO²
¹Institute of Materials Structure Science, High Energy Accelerator Organization (KEK), ²Materials Research Center for Element Strategy, Tokyo Institute of Technology, ³Comprehensive Research Organization for Science and Society, ⁴J-PARC Center, Japan Atomic Energy Agency

D2-11-P03

Nonlinear Current-Voltage Characteristics and High Permittivity in (In³⁺+Ta⁵⁺) Co-Doped TiO₂ Ceramics

 Prasit THONGBAI¹, Wattana TUICHAJ¹, Supamas DANWITTAYAKUL², Narong CHANLEK³
¹Khon Kaen University, ²National Metal and Materials Technology Center, ³Synchrotron Light Research Institute (Public Organization)

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 11–14, 2019

Symposium D-3

Science and Technology of Superconductivity

[Organizers]

Yoshihiko TAKANO (National Institute for Materials Science)
 Yoshikazu MIZUGUCHI (Tokyo Metropolitan university)
 Naurang SAINI (Sapienza University of Rome)
 Hai-Hu WEN (Nanjing University)

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December 11, 2019

Oral Session 1

Time 9:00–11:40 Room Trade-1

Chairpersons K. SHIMIZU, K. MATSUMOTO

Opening

9:00–9:10

D3-11-I01 ▶ Invited 9:10–9:40

Development of MgB₂ and (Ba,K)Fe₂As₂ Wires in NIMSHiroaki KUMAKURA¹, Zhaoshun GAO²,
Akiyoshi MATSUMOTO¹, Kazumasa TOGANO¹¹National Institute for Materials Science, ²Institute of
Electrical Engineering

D3-11-I02 ▶ Invited 9:40–10:00

Recent progress of high performance iron-based
superconducting wires

Yanwei MA

Institute of Electrical Engineering, Chinese Academy of
Sciences

D3-11-I03 ▶ Invited 10:00–10:20

Heteroepitaxial thin-film growth of iron-based
superconductors

Hidenori HIRAMATSU, Hideo HOSONO

Tokyo Institute of Technology

Coffee break

10:20–10:40

D3-11-I04 ▶ Invited 10:40–11:00

Electrical Transport Properties Of NdFeAs(O,F) Thin
Films On Vicinal Substrates

Kazumasa IIDA

Nagoya University

D3-11-I05 ▶ Invited 11:00–11:20

In-field and low temperature J_c properties of BHO
introduced Eu123 tapesSatoshi AWAJI¹, Tatsunori OKADA¹, Shinji FUJITA²,
Shogo MUTO², Wataru HIRATA², Yasuhiro IJIMA²,
Masanori DAIBO²¹IMR, Tohoku University, ²Fujikura co ltd.

D3-11-I06 ▶ Invited 11:20–11:40

Development of Processing Technology of Coated
Conductors to Contribute to Applications

Takato MACHI

AIST

December 11, 2019

Oral Session 2

Time 14:00–16:00 Room Trade-1

Chairperson S. AWAJI

D3-11-I07 ▶ Invited 14:00–14:20

High-Pressure Onset of High-Temperature
SuperconductivityKatsuya SHIMIZU¹, Mari EINAGA¹, Harushige NAKAO¹,
Masafumi SAKATA¹, Yuki NAKAMOTO¹, Akitaka NAKANISHI¹,
Takahiro ISHIKAWA^{1,2}, Saori KAWAGUCHI³, Naohisa HIRAO³,
Yasuo HIRAO³¹Osaka University, ²National Institute for Materials Science,
³JASRI

D3-11-I08 ▶ Invited 14:20–14:40

Ab initio study on the high temperature
superconductivity in compressed sulfur hydrides

Ryosuke AKASHI

The University of Tokyo

D3-11-I09 ▶ Invited 14:40–15:00

Search for Superconductivity of Hydrides synthesized
under High Pressure and High TemperatureMari EINAGA¹, Daichi TAKEDA¹, Masaomi KITAGAKI¹,
Harushige NAKAO¹, Masafumi SAKATA¹, Katsuya SHIMIZU¹,
Saori KAWAGUCHI², Naohisa HIRAO², Yasuo OHISHI²¹KYOKUGEN, Osaka University, ²JASRI

D3-11-I10 ▶ Invited 15:00–15:20

Data-driven Exploration for Pressure-induced Superconductors Using Novel Diamond Anvil Cell with Boron-doped Diamond Electrodes

 Ryo MATSUMOTO^{1,2}, Hou ZHUFENG³, Sayaka YAMAMOTO^{1,2}, Shintaro ADACHI¹, Masanori NAGAO⁴, Peng SONG^{1,2}, Yoshito SAITO^{1,2}, Takafumi D. YAMAMOTO¹, Kensei TERASHIMA¹, Hiromi TANAKA⁵, Tetsuo IRIFUNE⁶, Hiroyuki TAKEYA¹, Kiyoyuki TERAOKA^{1,7}, Yoshihiko TAKANO^{1,2}
¹National Institute for Materials Science, ²University of Tsukuba, ³Chinese Academy of Sciences, ⁴University of Yamanashi, ⁵National Institute of Technology, Yonago College, ⁶Ehime University, ⁷National Institute of Advanced Industrial Science and Technology

D3-11-I11 ▶ Invited 15:20–15:40

Search for Superconductivity in Compressed Hydrides by First-Principles Calculations and Evolutionary Algorithms

 Takahiro ISHIKAWA^{1,2}, Akitaka NAKANISHI², Katsuya SHIMIZU², Takashi MIYAKE³
¹ESICMM, National Institute for Materials Science, ²Center for Science and Technology under Extreme Conditions, Graduate School of Engineering Science, Osaka University, ³CD-FMat, National Institute of Advanced Industrial Science and Technology

D3-11-I12 ▶ Invited 15:40–16:00

Acceleration Search method of Higher T_c Superconductors by Machine Learning Algorithm

 Kaname MATSUMOTO, Tomoya HORIDE
Kyushu Institute of Technology

December 11, 2019

Oral Session 3
Time 16:30–18:30 **Room** Trade-1

Chairperson K. IIDA

D3-11-I13 ▶ Invited 16:30–16:50

Pressure-induced superconductivity in iron-based spin-ladder material BaFe_2S_3 and related materials

 Hiroki TAKAHASHI
Nihon University

D3-11-I14 ▶ Invited 16:50–17:10

Phenomena and physics related to superconductivity revealed by our recent high pressure studies

 Liling SUN¹, Jing GUO¹, Yazhou ZHOU¹, Qi WU¹, Tao XIANG¹, Robert CAVA², Guangming ZHANG³, Ni NI⁴
¹Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, ²Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA, ³State Key Laboratory for Low dimensional Quantum Physics and Department of Physics, Tsinghua University, Beijing 100084, China, ⁴Department of Physics and Astronomy, UCLA, Los Angeles, CA90095, USA

D3-11-I15 ▶ Invited 17:10–17:30

High-temperature superconductivity in ultrathin iron-chalcogenide films studied by angle-resolved photoemission spectroscopy

 Kosuke NAKAYAMA
Tohoku University

D3-11-I16 ▶ Invited 17:30–17:50

 EuFeAs_2 a 112-type Iron-pnictide: Novel Family of Magnetic Superconductors

 Michal BABIŃ, Lan Maria TRAN, Zbigniew BUKOWSKI
Institute of Low Temperature and Structure Research
Polish Academy of Sciences

D3-11-I17 ▶ Invited 17:50–18:10

A Review on a Functional Mixed Anion Layered Compound, $\text{Sr}_2\text{TMFeAsO}_{3-d}$ (TM: Transition Metals)

 Yoichi KAMIHARA
Keio University

D3-11-I18 ▶ Invited 18:10–18:30

Superconductivity in a New Iron Arsenide LaFe_2As_2

 Akira IYO¹, Shigeyuki ISHIDA¹, Hiroshi FUJIHISA¹, Yoshito GOTOH¹, Izumi HASE¹, Yoshiyuki YOSHIDA¹, Hiroshi EISAKI¹, Kenji KAWASHIMA^{1,2}
¹National Institute of Advanced Industrial Science and Technology (AIST), ²IMRA Material R&D Co., Ltd.

December 11, 2019

Poster Session
Time 19:00–20:30 **Room** Trade-0

D3-11-P01
Superconductivity in Bi-based layered superconductors

 Yoshikazu MIZUGUCHI
Tokyo Metropolitan University

D3-11-P02
Two-Fold-Symmetric Magnetization in Single Crystals of Tetragonal BiCh_2 -based Superconductor $\text{LaO}_{0.5}\text{F}_{0.5}\text{BiSSe}$

 Kazuhisa HOSHI¹, Motoi KIMATA², Tatsuma D MATSUDA¹, Yosuke GOTO¹, Toshikazu MIZUGUCHI¹
¹Tokyo Metropolitan University, ²Institute for Materials Research, Tohoku University

D3-11-P03
Crystal Size Improvement of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ Superconducting Whiskers Using Stress-controlled Precursors

 Sayaka YAMAMOTO^{1,2,3}, Ryo MATSUMOTO^{1,2}, Shintaro ADACHI², Yoshihiko TAKANO^{1,2}, Hiromi TANAKA³
¹University of Tsukuba, ²National Institute for Materials Science, ³National Institute of Technology, Yonago College

D3-11-P04**Chemical substitution effect in a possible topological superconductor**

Takeshi TAKAHASHI¹, Harald O. JESCHKE²,
Jun AKIMITSU², Kaya KOBAYASI^{1,2}

¹Department of Physics, Okayama University, ²RIIS,
Okayama University

D3-11-P05**Intra- and inter-granular superconducting properties and microstructure of BaFe₂As₂ polycrystalline bulks prepared by high energy milling**

Shinnosuke TOKUTA¹, Akiyasu YAMAMOTO¹,
Yusuke SHIMADA², Satoshi HATA³

¹Tokyo University of Agriculture and Technology, ²Tohoku
University, ³Kyushu University

D3-11-P06**Theoretical study of the uniaxial compression and tension effects on the superconductivity in two-leg ladder-type cuprates**

Hikaru SAKAMOTO, Kazuhiko KUROKI
University of Osaka

D3-11-P07**Vortex matter and dynamics in YBCO thin films with complex artificial pinning studied by DC magnetization, magnetic relaxation and AC susceptibility measurements**

Adrian CRISAN, Ion IVAN, Lucica MIU
National Institute for Materials Physics

D3-11-P08**Superconducting Thin Films of Bi₂Sr₂CaCu₂O_{8+x} for Future THz Planar Devices**

Kazuhiro ENDO¹, Shunichi ARISAWA², Petre BADICA³

¹Kanazawa Institute of Technology, ²National Institute for
Materials Science, ³National Institute of Materials Physics

D3-11-P09**Unconventional Superconductivity Properties of Re Doped Weyl Semimetal MoTe₂**

Ravi Prakash SINGH, Manasi MANDAL, Saurav MARIK

Indian Institute of Science Education and Research Bhopal,
Bhopal, 462066, India

D3-11-P10**Epitaxial Stabilization and Electrochemical Doping Make Metastable Titanates New Superconducting Materials**

Akira OHTOMO^{1,2}, Kohei YOSHIMATSU¹

¹Department of Chemical Science and Engineering, Tokyo
Institute of Technology, ²Materials Research Center for
Element Strategy, Tokyo Institute of Technology

D3-11-P11**The First Discovery of superconductivity in Yb-based compounds YbTr₂Al₂₀ (Tr = Mo, Ta)**

Naoki NAKAMURA¹, Ryuji HIGASHINAKA¹, Yuji AOKI¹,
Hideyuki SATO¹, Dai AOKI², Tatsuma D. MATSUDA¹

¹Tokyo Metropolitan University, ²Tohoku University

D3-11-P12**Growth and superconducting transition temperature of (La,Ce)OBiS₂ single crystals**

Yuji HANADA¹, Masanori NAGAO¹, Akira MIURA²,
Yuki MARUYAMA¹, Satoshi WATAUCHI¹,
Yoshihiko TAKANO³, Isao TANAKA¹

¹University of Yamanashi, ²Hokkaido University, ³National
Institute for Materials Science

D3-11-P13**Superconducting properties of RE123 superconductor with high-entropy-alloy-type RE site**

Yuta SHUKUNAMI

Tokyo Metropolitan University

D3-11-P14**New Types Of Iron-Oxypnictide Heterostructures And Their Interfaces**

Silvia HAINDL¹, Masato SASASE², Hidenori HIRAMATSU²,
Hideo HOSONO^{2,3}, Erik KAMPERT⁴, Ian MACLAREN⁵

¹World Research Hub Initiative, Institute of Innovative
Research, Tokyo Institute of Technology, ²Materials
Research Center for Element Strategy, Tokyo Institute
of Technology, ³Laboratory for Materials and Structures,
Institute of Innovative Research, Tokyo Institute of
Technology, ⁴Dresden High Magnetic Field Laboratory
(HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf,
⁵School of Physics and Astronomy, University of Glasgow

D3-11-P15**Hydrogen annealing effect of superconducting properties in FeSe_{1-x}Te_x**

Daiki YAMANE¹, Kazumasa HORIGANE², Jun AKIMITSU²

¹Graduate School of natural science and technology,
Okayama University, ²Research Institute for Interdisciplinary
Science, Okayama University

D3-11-P16**Superconducting Critical Current Density Enhanced to 285 A cm⁻² for Sr₂VFeAsO_{3.6} Tape Fabricated via ex-situ Powder-in-tube Process**

Suguru IWASAKI¹, Ryo MATSUMOTO², Shintaro ADACHI²,
Yoshihiko TAKANO², Yoichi KAMIHARA¹

¹Keio, ²NIMS

D3-11-P17**Broken time-reversal symmetry probed by muon spin relaxation in the caged type superconductors R₅Rh₆Sn₁₈ (R = Lu, Sc, Y)**

Devashibhai Thakarshibhai ADROJA

Rutherford Appleton Laboratory

D3-11-P18**Synthesis of the Mother Phase of the Iron-Based Superconductor SmFeAsO at Low Temperatures**

Ryosuke SAKAGAMI¹, Simon R. HALL², Jason POTTICARY²,
Masanori MATOBA¹, Yoichi KAMIHARA¹

¹Keio University, ²University of Bristol

D3-11-P19

 Crystal structure and superconducting properties of $Sr_{1-x}RE_xFBiS_2$ ($RE: La, Ce, Pr, Nd, Sm$) BiS_2 -based layered superconductors

 Aichi YAMASHITA, Yoshikazu MIZUGUCHI
 Tokyo Metropolitan University

D3-11-P20

 Superconductivity at 4 K for Eu doped $La_{2-x}Eu_xO_2Bi_3Ag_{0.6}Sn_{0.4}S_6$

 RAJVEER JHA
 Tokyo Metropolitan University

D3-11-P21

Control of the physical property by the field effect diamond anvil cell

 Yoshihiko TAKANO^{1,2}, Shintaro ADACHI¹
¹National Institute for Materials Science (NIMS), ²Tsukuba Univ.

D3-11-P22

 Superconducting Joints between $Bi2223$ and $NbTi$ Wires using $Bi-Pb-Sn$ Solder

 Yoshihiko TAKANO^{1,2}, Kazuo INOUE¹
¹National Institute for Materials Science (NIMS), ²Tsukuba Univ.

December 12, 2019

Oral Session 4

Time 9:00–12:10 Room Work-1

Chairpersons K. TANIGAKI, T. YOKOYA

D3-12-I01 ▶ Invited

9:00–9:30

Neutron Irradiation: from Single Displaced Atoms to Nanometer Sized Defects and their Influence on Superconductivity in Various Materials

 Michael EISTERER¹, David X. FISCHER¹, Daniel KAGERBAUER¹, Raphael UNTERRAINER¹, Thomas BAUMGARTNER¹, Stephan PFEIFFER², Johannes BERNARDI²
¹TU Wien, Atominstytut, ²TU Wien, USTEM

D3-12-I02 ▶ Invited

9:30–9:50

Vortex dynamics of REBCO films irradiated with low-energy ion irradiations

 Toshinori OZAKI
 Kwansai Gakuin University

D3-12-I03 ▶ Invited

9:50–10:10

Effect of ion irradiation on cuprate and iron-based superconductors

 Qiang LI
 Brookhaven National Laboratory

D3-12-I04 ▶ Invited

10:10–10:30

 Extraordinary pinning efficiency of one-dimensional artificial pinning centers with coherent interfaces in $YBa_2Cu_3O_{7-x}$ nanocomposite films

 Judy WU
 University of Kansas

 Coffee break
 10:30–10:50

D3-12-I05 ▶ Invited

10:50–11:10

Designed nano-structures in high performance oxide superconducting films controlled by novel PLD growth techniques

 Yutaka YOSHIDA¹, Yusuke ICHINO¹, Yuji TSUCHIYA¹, Tomohiro ITO¹, Kaname MATSUMOTO², Ataru ICHINOSE³, Satoshi AWAJI⁴
¹Nagoya University, ²Kyushu Inst. Tech., ³Central Research Institute of Electric Power Industry, ⁴Tohoku University

D3-12-I06 ▶ Invited

11:10–11:30

 Possibility of Unconventional High- T_c Superconductivity Originating from Coexisting Wide and Narrow Bands

 Kazuhiko KUROKI
 Osaka University

D3-12-I07 ▶ Invited

11:30–11:50

 Electronic compressibility and high- T_c superconductivity: new links

 Luca DE MEDICI
 ESPCI

D3-12-I08 ▶ Invited

11:50–12:10

 High- T_c cuprates – story of two electronic subsystems

 Neven BARISIC^{1,2}
¹TU Wien, ²PMF Zagreb

December 12, 2019

Cluster Session D

Time 14:00–16:00 Room Ken-1

Chairpersons Yoshihiro Iwasa, Kenji Shiojima, Susumu Saito

DX-12-CLK01

14:00–14:40

Atomic-level control of high temperature superconductor materials for unveiling their pairing mechanism

 Qi-kun XUE
 Tsinghua University, China

DX-12-CLK02

14:40–15:20

Development of Corundum-Structured Gallium Oxide Power Devices by MIST EPITAXY®

 Takashi SHINOHE
 FLOSFIA INC., Japan.

DX-12-CLK03 15:20–16:00

Emergent electromagnetism in quantum materialsNaoto NAGAOSA
RIKEN and U. Tokyo, Japan

December 12, 2019

Oral Session 6

Time 16:30–18:30 Room Work-1

Chairperson K. KUROKI

Symposium special talk

What value can ebook bring in?

~Case in materials science~

Akiyuki Tokuno

Editor, Books, Science, Springer

16:30–16:50

D3-12-I09 ▶ Invited 16:50–17:10

High-resolution photoelectron holography of heavily boron-doped diamondTakayoshi YOKOYA¹, Wataru HOSODA¹, Takumi TANIGUCHI¹, Kensei TERASHIMA¹, Hirokazu FUJIWARA¹, Yuko YANO¹, Tomohiro MATSUSHITA², Takayuki MURO², Toyohiko KINOSHITA², Yoshihiko TAKANO³, Taisuke KAGEURA⁴, Hiroshi KAWARADA⁴, Tamio OGUCHI⁵, Yuji MURAOKA¹¹Okayama University, ²Japan Synchrotron Radiation Research Institute, ³National Institute for Materials Science, ⁴Waseda University, ⁵Osaka University

D3-12-I10 ▶ Invited 17:10–17:30

Fundamental Properties and Device Applications of Superconducting Single-crystalline Boron-doped DiamondTaisuke KAGEURA^{1,2}, Yoshihiko TAKANO², Hiroshi KAWARADA^{2,3}¹National Institute for Materials Science, ²Waseda University, ³The Kagami Memorial Laboratory for Materials Science and Technology Waseda University

D3-12-I11 ▶ Invited 17:30–17:50

High Pressure Polymerization of Metal Doped C₆₀ ~In an Attempt to Prepare Carbon Clathrate High T_c Superconductor~Masashi TANAKA
Kyushu Institute of Technology

D3-12-I12 ▶ Invited 17:50–18:10

Electron-Phonon and Electron-Electron Interactions in Electron Doped Aromatic Carbon Materials viewed from Electrical TransportKatsumi TANIGAKI, Yuki MATSUDA
Tohoku University

D3-12-I13 ▶ Invited 18:10–18:30

Enhanced Superconductivity in Polar IV – VI SemiconductorsMarkus KRIENER¹, M. KAMITANI¹, T. KORETSUNE^{1,2}, S. M. BAHRAMY^{1,3}, M. SAKANO³, R. YUKAWA⁴, K. HORIBA⁴, H. KUMIGASHIRA⁴, K. ISHIZAKA^{1,3}, R. ARITA^{1,3}, Y. TOKURA^{1,3}, Y. TAGUCHI¹¹RIKEN Center for Emergent Matter Science (CEMS), Wako 351-0198, Japan, ²Department of Applied Physics and Quantum-Phase Electronics Center (QPEC), University of Tokyo, Tokyo 113-8656, Japan, ³Photon Factory, Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK), Tsukuba, Ibaraki 305-0801, Japan

December 13, 2019

Oral Session 7 (1)

Time 9:00–12:10 Room Work-1

Chairpersons H. KUMAKURA, M. EISTERER

D3-13(1)-I01 ▶ Invited 9:00–9:30

Emerging materials for high field applications: activities at CNR-SPIN.Carlo FERDEGHINI¹, Emilio BELLINGERI¹, Cristina BERNINI¹, Valeria BRACCINI¹, Alessandro LEVERATTO¹, Andrea MALAGOLI¹, Pietro MANFRINETTI^{1,2}, Ilaria PALLECCHI¹, Alessia PROVINO¹, Marina PUTTI^{1,2}, Aisha SABA^{1,2}, Giulia SYLVA^{1,2}, Andrea TRAVERSO^{1,2}¹CNR-SPIN, Genova, Italy, ²University of Genova, Italy

D3-13(1)-I02 ▶ Invited 9:30–9:50

Magnetic Properties in Superconducting Metals and Alloys Processed by High-Pressure TorsionTerukazu NISHIZAKI¹, Kaveh EDALATI^{2,3}, Seungwon LEE⁴, Zenji HORITA^{2,3}, Tadahiro AKUNE¹, Tsutomu NOJIMA⁵, Satoshi IGUCHI⁵, Takahiko SASAKI⁵¹Department of Electrical Engineering, Kyushu Sangyo University, ²WPI, International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, ³Department of Materials Science and Engineering, Kyushu University, ⁴Department of Materials Design and Engineering, University of Toyama, ⁵Institute for Materials Research, Tohoku University

D3-13(1)-I03 ▶ Invited 9:50–10:10

Recent Progress in Nb₃Sn High Field Performance

Chiara TARANTINI, Shreyas BALACHANDRAN, Peter L. LEE, Fumitake KAMETANI, Yi-Feng SU, Benjamin WALKER, William L. STARCH, David C. LARBALESTIER

Applied Superconductivity Center, National High Magnetic Field Laboratory, Florida State University

D3-13(1)-I04 ▶ Invited 10:10–10:30

Development of MgB₂-based Materials Towards Different Superconducting ApplicationsPetre BADICA
National Institute of Materials Physics

[Coffee break
10:30–10:50]

D3-13(1)-I05 ▶ Invited 10:50–11:10

Monolithic terahertz emitter of high-temperature superconductors

Itsuhiro KAKAYA¹, Asem ELARABI¹, Keiichiro MAEDA¹, Shuma FUJITA¹, Manabu TSUJIMOTO²

¹Kyoto University, ²University of Tsukuba

D3-13(1)-I06 ▶ Invited 11:10–11:30

Development of High- T_c Superconducting THz Emitters

Takanari KASHIWAGI^{1,2}, Shungo NAKAGAWA¹, Takayuki IMAI¹, Genki KUWANO¹, Youta KANEKO¹, Yukino ONO¹, Shinji KUSUNOSE¹, Takashi YAMAMOTO³, Hidetoshi MINAMI^{1,2}, Manabu TSUJIMOTO^{1,2}, Kazuo KADOWAKI⁴

¹Graduate School of Pure & Applied Sciences, University of Tsukuba, ²Division of Materials Science, Faculty of Pure & Applied Sciences, University of Tsukuba, ³QuTech, Delft University of Technology, ⁴Algae Biomass and Energy System R&D Center, University of Tsukuba

D3-13(1)-I07 ▶ Invited 11:30–11:50

Elemental Substitution in the RE-123 and Bi-2212 Cuprate Superconductors for the Enhancement of T_c .

Masatsune KATO, Kohei NAKAGAWA, Takayuki KAWAMATA, Takashi NOJI, Yoji KOIKE

Tohoku University

D3-13(1)-I08 ▶ Invited 11:50–12:10

Bond vs. Diagonal Nematicity in the Pseudogap Phase of High-Temperature Cuprate Superconductors

Shigeru KASAHARA

Kyoto University

December 13, 2019

Oral Session 7 (2)

Time 9:00–12:10 Room Work-6

Chairpersons R. ARITA

D3-13(2)-I01 ▶ Invited 10:50–11:10

Polymorphism and Superconductivity in Platinum Pnictides

Minoru NOHARA

Okayama University

D3-13(2)-I02 ▶ Invited 11:10–11:30

Pressure-induced superconductivity in non-symmorphic CrAs

Hisashi KOTEGAWA

Kobe University

D3-13(2)-I03 ▶ Invited 11:30–11:50

Unconventional Superconductivity in Noncentrosymmetric Superconductors

Ravi Prakash SINGH

IISER Bhopal

D3-13(2)-I04 ▶ Invited 11:50–12:10

Possible valence skipping superconductivity in doped Dirac metal

Kaya KOBAYASHI^{1,2}, T. UENO¹, T. WAKITA², T. FURUKAWA³, T. ITOU³, T. YOKOYA^{1,2}, J. AKIMITSU²

¹Department of Physics, Okayama University, ²RIIS, Okayama University, ³Department of Applied Physics, Tokyo University of Science

December 13, 2019

Oral Session 8 (1)

Time 14:00–16:00 Room Work-1

Chairperson C. FERDEGHINI

D3-13(1)-I09 ▶ Invited 14:00–14:20

Novel Electronic Nematicity in Heavily Hole-Doped Iron-Pnictide Superconductors

Takasada SHIBAUCHI

University of Tokyo

D3-13(1)-I10 ▶ Invited 14:20–14:40

The Interplay of Superconductivity and Magnetism in Iron Based Superconductors: Study of EuFe₂As₂-based Magnetic-Superconductors

Lan Maria TRAN, Michał BABIŁ, Zbigniew BUKOWSKI, Andrzej J. ZALESKI

Institute of Low Temperature and Structure Research Polish Academy of Sciences in Wrocław

D3-13(1)-I11 ▶ Invited 14:40–15:00

Superconducting properties of 1144-type iron pnictide superconductors

Hiraku OGINO¹, Shigeyuki ISHIDA¹, Akira IYO¹, Hiroshi EISAKI¹, Kenji KAWASHIMA^{1,2}

¹National Institute of Advanced Industrial Science and Technology (AIST), ²IMRA Material R&D Co., Ltd.

D3-13(1)-I12 ▶ Invited 15:00–15:20

Quasi-particle self-consistent GW calculations and superconductivity in iron-based Superconductors

Katsuhiro SUZUKI¹, Taishi OGURA², Hirofumi SAKAKIBARA^{3,4}, Takao KOTANI³, Hiroaki IKEDA²

¹Research Organization of Science and Technology, Ritsumeikan University, ²Department of Physics, Ritsumeikan University, ³Department of Applied Mathematics and Physics, Tottori University, ⁴Computational Condensed Matter Physics Laboratory

D3-13(1)-I13 ▶ Invited 15:20–15:40

Magnetism in Fe pnictides and chalcogenides

Rudi HACKL

Walther Meissner Institut, Bayerische Akademie der Wissenschaften

D3-13(1)-I14 ▶ Invited 15:40–16:00
 μ SR Study of Multigap Superconductivity in
 $ACa_2Fe_4As_4F_2$ (A = K, Rb and Cs)
 Devashibhai Thakarshibhai ADROJA
 Rutherford Appleton Laboratory

December 13, 2019
Oral Session 8 (2)
 Time 14:00–16:00 Room Work-6
 Chairperson K. KOBAYASHI

D3-13(2)-I05 ▶ Invited 14:00–14:20
 Chiral Majorana Mode in Topological Superconducting
 Element hcp Thallium
 Ryotaro ARITA^{1,2}
¹University of Tokyo, ²RIKEN Center for Emergent Matter
 Science

D3-13(2)-I06 ▶ Invited 14:20–14:40
 Zero-energy modes in topological materials:
 experimental observations and proposed models
 Tomasz DIETL
 International Research Centre MagTop, Institute of Physics,
 Polish Academy of Sciences

D3-13(2)-I07 ▶ Invited 14:40–15:00
 Observation and control of nematic topological
 superconductivity in doped Bi_2Se_3 superconductors
 Shingo YONEZAWA
 Kyoto University

D3-13(2)-I08 ▶ Invited 15:00–15:20
 NMR studies of Topological Superconductors
 Kazuaki MATANO
 Okayama University

D3-13(2)-I09 ▶ Invited 15:20–15:40
 Nature of zero-energy vortex bound state in
 superconducting topological surface state of $Fe(Se,Te)$
 Tadashi MACHIDA
 RIKEN

D3-13(2)-I10 ▶ Invited 15:40–16:00
 Superconductivity and Possible Electronic Nematic
 Phases in Titanium Pnictide Oxides
 Takeshi YAJIMA¹, Wataru ISHII¹, Shunsaku KITAGAWA²,
 Kenji ISHIDA², Kota KATAOKA¹, Kanako TAKAHASHI¹,
 Zenji HIROI¹
¹University of Tokyo, ²Kyoto University

December 13, 2019
Oral Session 9 (1)
 Time 16:30–18:30 Room Work-1
 Chairperson I. KAKEYA

D3-13(1)-I15 ▶ Invited 16:30–16:50
 Growth and evaluation of multi rare earth elements
 substituted $ROBiS_2$ (R: rare earth elements)
 superconducting single crystals
 Masanori NAGAO¹, Yuji HANADA¹, Akira MIURA²,
 Yuki MARUYAMA¹, Satoshi WATAUCHI¹,
 Yoshihiko TAKANO³, Isao TANAKA¹
¹University of Yamanashi, ²Hokkaido University, ³National
 Institute for Materials Science

D3-13(1)-I16 ▶ Invited 16:50–17:10
 Bulk superconductivity induced via two-site
 substitution in $La_2O_2M_4S_6$ -type layered oxychalcogenide
 $La_2O_2Bi_3Ag_{0.6}Sn_{0.4}S_{5.7}Se_{0.3}$
 RAJVEER JHA, Yosuke GOTO, Yoshikazu MIZUGUCHI
 Tokyo Metropolitan University

D3-13(1)-I17 ▶ Invited 17:10–17:30
 The change of electronic structure by Bi dimer disconnection
 in the bismuth chalcogenide superconductor $CsBi_{4-x}Pb_xTe_6$
 Hiroyuki OKAZAKI^{1,2,3}, Kensei TERASHIMA³,
 David BILLINGTON⁴, Takanori WAKITA², Yoshihiko TAKANO³,
 Yuji MURAOKA², Takayoshi YOKOYA²
¹Takasaki Advanced Radiation Research Institute, National
 Institutes for Quantum and Radiological Science and
 Technology, ²Research Institute for Interdisciplinary Science
 (RIIS), Okayama University, ³National Institute for Materials
 Science, ⁴School of Physics and Astronomy, Cardiff University

D3-13(1)-I18 ▶ Invited 17:30–17:50
 Scanning Tunneling Microscopy/Spectroscopy Study in
 $BiCh_2$ superconductors
 Satoshi DEMURA¹, Shotaro SHOBU², Kazuki MIYATA²,
 Shin-ichi KANEKO³, Satoshi OKUMA³
¹Nihon University, ²Tokyo University of Science, ³Tokyo
 Institute of Technology

D3-13(1)-I19 ▶ Invited 17:50–18:10
 Study of chemical pressure effect on electronic- and
 local crystal-structure in $LaOBiCh_2$ system
 Kensei TERASHIMA¹, Yuko YANO², Eugenio PARIS³,
 Yosuke GOTO⁴, Yoshikazu MIZUGUCHI⁴, Yoichi KAMIHARA⁵,
 Takanori WAKITA⁶, Yuji MURAOKA⁶, Naurang L. SAINI³,
 Takayoshi YOKOYA⁶
¹National Institute for Materials Science, ²Graduate School
 of Natural Sciences, Okayama University, ³Department of
 Physics, University of Rome "La Sapienza", ⁴Department
 of Physics, Tokyo Metropolitan University, ⁵Department of
 Applied Physics and Physico-Informatics, Keio University,
⁶Research Institute for Interdisciplinary Science, Okayama
 University

Symposium special talk
 18:10–18:30

December 13, 2019
Oral Session 9 (2)

Time 16:30–18:30 Room Work-6

Chairperson H. KOTEGAWA

D3-13(2)-I11 ▶ Invited 16:30–16:50

Spin-Triplet Superconductivity and Field-Induced Phenomena in Uranium Compounds

Dai AOKI

IMR, Tohoku University

D3-13(2)-I12 ▶ Invited 16:50–17:10

NMR Studies on U-based Ferromagnetic Superconductors

Kenji ISHIDA

Kyoto University

D3-13(2)-I13 ▶ Invited 17:10–17:30

 NMR studies of Spin-Triplet Superconductors UPt_3 and UBe_{13} : An Aspect of Spin-Orbit Interaction Experienced by the Cooper

Hideki TOU

Department of Physics, Kobe University

D3-13(2)-I14 ▶ Invited 17:30–17:50

The First Discovery of Superconducting State and Fermi Surface Properties in Yb-based Skutterudite and 1-2-20 Systems

Tatsuma D. MATSUDA

Tokyo Metropolitan University

D3-13(2)-I15 ▶ Invited 17:50–18:10

 Material Design of Light Rare-Earth Dodecaborides by High Pressure Synthesis and Novel Feature of Kondo Insulator YbB_{12}

 Fumitoshi IGA¹, Wataru MATSUHARA¹, Hiroyuki NAKAYAMA¹, Takahiro YAMADA¹, Hyohma TAKEMORI¹, Akira MATSUO², Yasuhiro H. MATSUDA², Yoshimitsu KOHAMA², Koichi KINDO², Toru SHIMMEI³, Takehiro KUNIMOTO³, Tetsuo IRIFUNE³, Norimasa NISHIYAMA⁴, Hitoshi SATO⁵, Tomoko KAGAYAMA⁶, Katsuya SHIMIZU⁶
¹Institute of Quantum Beam Science, Ibaraki University,

²Institute of Solid State Physics, University of Tokyo,

³Geodynamics Research Center, Ehime University,

⁴Laboratory for Materials and Structures, Tokyo Institute of Technology,

⁵Hiroshima Synchrotron Radiation Center, Hiroshima University,

⁶Center for Science and Technology under Extreme Conditions, Osaka University

D3-13(2)-I16 ▶ Invited 18:10–18:30

 Multipole ordering in a Pr-based quaternary compound $PrRu_2Sn_2Zn_{18}$

 Kazuhei WAKIYA¹, Takahiro KOMAGATA¹, Yuki SUGIYAMA¹, Masatomo UEHARA¹, Jun GOUCHI², Kazuyuki MATSUBAYASHI³, Yoshiya UWATOKO², Izuru UMEHARA¹
¹Yokohama National University, ²The University of Tokyo,

³The University of Electro-Communications

December 14, 2019

Oral Session 10

Time 9:00–12:20 Room Work-1

Chairpersons Y. TAKANO, Y. MIZUGUCHI

D3-14-I01 ▶ Invited 9:00–9:30

Science and Technology on Recent Bi2223 Joints Connecting DI-BSCCO

 Jun-ichi SHIMOYAMA¹, Yasuaki TAKEDA², Takanori MOTOKI¹, Takayoshi NAKASHIMA³, Shin-ichi KOBAYASHI³, Takeshi KATO³
¹Aoyama Gakuin University, ²The University of Tokyo,

³Sumitomo Electric Industries

D3-14-I02 ▶ Invited 9:30–9:50

Overview of the performance test of 1km-long high-Tc superconducting DC cable system in Ishikari and future prospects

Noriko CHIKUMOTO, Hirofumi WATANABE, Yury IVANOV, Satarou YAMAGUCHI

Center of Applied Superconductivity and Sustainable Energy Research, Chubu University

D3-14-I03 ▶ Invited 9:50–10:10

Grain Boundary structures and Intergrain Connectivity in Bi-2212 and Ba-122 High Temperature Superconductors

Fumitake KAMETANI, Yavuz OZ, Abiola OLOYE, Chongin PAK, Shah LIMON, Yi-Feng SU, Jianyi JIANG, Ulf TROCIEWITZ, Chiara TARANTINI, Eric HELLSTROM, David LARBALESTIER

Florida State University

D3-14-I04 ▶ Invited 10:10–10:30

Exploring Ternary Molybdenum Superconducting Nitrides by Self-Combustion Synthesis

 Akira MIURA¹, Jin ODAHARA¹, Nataly Carolina ROSERO-NAVARRO¹, Masanori NAGAO², Isao TANAKA², Kiyoharu TADANAGA¹
¹Hokkaido University, ²University of Yamanashi

 [Coffee break
10:30–10:50]

D3-14-I05 ▶ Invited 10:50–11:10

Solid state electrochemistry for intercalation by using proton-driven ion introduction

 Masaya FUJIOKA¹, Kento SATO¹, Masanori NAGAO², Satoshi DEMURA³, Hideaki SAKATA⁴, Shintaro ADACHI⁵, Yoshihiko TAKANO⁵, Hideo KAIJU⁶, Melbert JEEM¹, Junji NISHII¹
¹Hokkaido University, ²University of Yamanashi, ³Nihon

 University, ⁴Tokyo University of Science, ⁵National Institute

 for Materials Science, ⁶Keio University

D3-14-I06 ▶ Invited 11:10–11:30

Layered Tin Pnictides as a New Class of van der Waals-type Superconductors

Yosuke GOTO

Tokyo Metropolitan University

D3-14-I07 ▶ Invited 11:30–11:50

Exploring novel superconductors in low-dimensional materials

Zhi An REN

Institute of Physics, Chinese Academy of Sciences

D3-14-I08 ▶ Invited 11:50–12:10

Carrier-doping to Iridate Sr_2IrO_4

Jun AKIMITSU

Okayama University

[Closing 12:10–12:20]

December 11–12, 2019

Symposium D-4

5th E&J BLS

Wide-bandgap and 2-dimensional Materials

[Organizers]

Kenji SHIOJIMA (University of Fukui)
 Fumimasa HORIKIRI (SCIOCS Co. Ltd.)
 Hiroshi KAWARADA (Waseda University)
 Akihiro HASHIMOTO (University of Fukui)
 Patrick CHIN (Intelligent Epitaxy Technology Inc.)
 Matteo MENEGHINI (Padova Univ.)

December 11, 2019

Oral Session 1

Time 9:00–11:30 Room Trade-3

Chairperson Kenji SHIOJIMA

 Blank
 9:00–9:30

D4-11-I01 ▶ Invited 9:30–10:00

Reliability and Dynamic Performance of Gallium Nitride-based Devices for Power Applications

Carlo DE SANTI, Matteo MENEGHINI,
 Alessandro BARBATO, Matteo BORGA, Eleonora CANATO,
 Francesca CHIOCCHETTA, Elena FABRIS, Zhan GAO,
 Fabrizio MASIN, Kalparupa MUKHERJEE, Arianna NARDO,
 Maria RUZZARIN, Mehdi RZIN, Alaleh TAJALLI,
 Gaudenzio MENEGHESSO, Enrico ZANONI
 University of Padova

D4-11-I02 ▶ Invited 10:00–10:30

Ultra-wide Bandgap Al-rich AlGa_N Alloys for Power Diodes and Transistors

Andrew ALLERMAN, Mary H. CRAWFORD,
 Andrew M. ARMSTRONG, Greg W. PICKRELL,
 Jeremy R. DICKERSON, Robert J. KAPLAR,
 Andrew T. BINDER, Michael L. SMITH, Vincent M. ABATE
 Sandia National Laboratories

D4-11-I03 ▶ Invited 10:30–11:00

Effects of device structures and epi properties on high efficiency AlGa_N/Ga_N HEMTs

Kazutaka TAKAGI, Kenichi SUGITA, Kunio TSUDA,
 Hideki KIMURA
 Toshiba Infrastructure Systems & Solutions Corporation

D4-11-I04 ▶ Invited 11:00–11:30

Compositional metrology of Atom Probe Tomography applied to III-N optoelectronic devices

Lorenzo RIGUTTI
 University of Rouen Normandie, Groupe de Physique des Matériaux

December 11, 2019

Oral Session 2

Time 14:00–16:00 Room Trade-3

Chairpersons Patrick CHIN, Kenji SHIOJIMA

D4-11-I05 ▶ Invited 14:00–14:30

The Hunt for Mobile Holes Induced by Polarization in GaN

Huili Grace XING
 Cornell University

D4-11-I06 ▶ Invited 14:30–15:00

Challenge and Opportunity for Mass Production of UVC LED by MOVPE on High Temperature Annealed AlN Template

Koh MATSUMOTO¹, Yuji TOMITA¹, Akira MISHIMA¹,
 Yuya YAMAOKA¹, Shuuichi KOSEKI¹, Yoshiki YANO¹,
 Hideto MIYAKE², Hideki HIRAYAMA³
¹TAIYO NIPPON SANCO, ²Mie University, ³RIKEN

D4-11-I07 ▶ Invited 15:00–15:30

Breakdown Phenomena in High- and Low-Voltage SiC Devices

Tsunenobu KIMOTO
 Kyoto University

D4-11-I08 ▶ Invited 15:30–16:00

Carrier Recombination Velocity in 4H-SiC: at Surfaces and Defects

Masashi KATO
 Nagoya Institute of Technology

December 11, 2019

Oral Session 3

Time 16:30–18:30 Room Trade-3

Chairperson Matteo MENEGHINI

D4-11-I09 ▶ Invited 16:30–17:00

Vertical GaN p-n Junction Diodes Fabricated on Free-standing GaN Substrates

Tomoyoshi MISHIMA
 Hosei University

D4-11-I10 ▶ Invited 17:00–17:30

GaN-based normally-off HEMTs for switching and logic applications

Jan KUZMIK
 Institute of Electrical Eng., Slovak Academy of Sci.

D4-11-I11 ▶ Invited 17:30–18:00

Ab-initio based description and design of nitride surfaces: The role of surface rehybridization on alloy composition and ordering.

Liverios LYMPERAKIS, Christoph FREYSOLDT, Jörg NEUGEBAUER

Computational Materials Design departement, Max-Planck-Institut für Eisenforschung

D4-11-I12 ▶ Invited 18:00–18:30

Epitaxial Growth of N-Polar Nitride Semiconductor and its Device Application

Takashi MATSUOKA

New Industry Creation Hatchery Center, Tohoku University

December 12, 2019

Oral Session 4

Time 9:00–11:30 Room Miel-5

Chairperson Fumimasa HORIKIRI

[Blank
9:00–10:00]

D4-12-I01 ▶ Invited 10:00–10:30

Electrochemical application on boron-doped diamond electrodes

Yasuaki EINAGA

Keio University

D4-12-I02 ▶ Invited 10:30–11:00

Electrical properties of GaN MOS capacitors with ALD-High-k gate insulators

Toshihide NABATAME¹, Yoshihiro IROKAWA¹, Koji SHIOZAKI², Yasuo KOIDE¹

¹National Institute for Materials Science, ²Institute of Materials and Systems for Sustainability, Nagoya University

D4-12-003 11:00–11:15

Difference in carrier lifetimes for SiC measured by microwave photoconductivity decay and time-resolved photoluminescence methods

Masashi KATO

Nagoya Institute of Technology

D4-12-004 11:15–11:30

Simple Photoelectrochemical Etching of GaN for RF Application

Fumimasa HORIKIRI¹, Noboru FUKUHARA¹, Yoshinobu NARITA¹, Takehiro YOSHIDA¹, Masachika TOGUCHI², Kazuki MIWA², Taketomo SATO²

¹SCIOCS Company Limited, ²Hokkaido University

December 12, 2019

Oral Session 6

Time 16:30–18:30 Room Work-6

Chairperson Akihiro HASHIMOTO

D4-12-I05 ▶ Invited 16:30–17:00

Structural evaluation of β -Ga₂O₃ crystals by TEM and related techniques

Osamu UEDA¹, Akito KURAMATA², Hiroataka YAMAGUCHI³, Makoto KASU⁴

¹Meiji University, ²Novel Crystal Technology Inc., ³National Institute of Advanced Industrial Science and Technology, ⁴Saga University

D4-12-I06 ▶ Invited 17:00–17:30

Photoemission Study of Chemically-Cleaned GaN Surfaces and GaN-SiO₂ Interfaces Formed by Remote Plasma CVD

Seiichi MIYAZAKI, Akio OHTA

Nagoya University

D4-12-I07 ▶ Invited 17:30–18:00

Fabrication and characterization of twisted bilayer graphene

Satoru TANAKA¹, Hitoshi IMAMURA¹, Ryo-suke UOTANI¹, Takashi KAJIWARA¹, Anton VISIKOVSKIY¹, Takushi IIMORI², Toshio MIYAMACHI², Kan NAKATSUJI³, Kazuhiko MASE⁴, Fumio KOMORI²

¹Kyushu Univ., ²Univ. Tokyo, ³Tokyo Inst. Tech., ⁴KEK

D4-12-008 18:00–18:15

New Method for First-principles Electronic-structure Study of Impurity Induced States and its Application to Diamond and Cubic BN

Hiroki YAMASHITA¹, Taishi HAGA¹, Yoshitaka FUJIMOTO¹, Susumu SAITO^{1,2,3}

¹Department of Physics, Tokyo Institute of Technology, ²Advanced Research Center for Quantum Physics and Nanoscience, Tokyo Institute of Technology, ³Materials Research Center for Element Strategy, Tokyo Institute of Technology

D4-12-009 18:15–18:30

High electrical conductivity exceeding ~ 3000 S cm⁻¹ of a transparent oxide semiconductor, La-doped SrSnO₃

Mian WEI¹, Anup V. SANCHELA², Hai Jun CHO^{1,2}, Hiromichi OHTA^{1,2}

¹Graduate School of Information Science and Technology, Hokkaido University, ²Research Institute for Electronic Science, Hokkaido University



December 11, 2019

Poster Session

Time 19:00–20:30 Room Trade-0

D4-11-P01

Repair of Multifunctional Two Dimension Structure by Additional Growth of AlN Atomic Layer in MEE Mode

Yuta KAMADA, Tomoya TAKEUCHI, Riku SHAMOTO,
Akihiro HASHIMOTO
University of Fukui

D4-11-P02

Orientation Control of a-axis in InN Growth by AlN/ Epitaxial Graphene/4H-SiC(0001)

Riku SHAMOTO, Yuta KAMADA, Akihiro HASHIMOTO
University of Fukui

D4-11-P03

Mapping of Photo-Electrochemical Etched Ni/ n-GaN Schottkey Contacts Using Scanning Internal Photoemission Microscopy

Ryo MATSUDA¹, Fumimasa HORIKIRI²,
Yoshinobu NARITA², Takehiro YOSHIDA²,
Tomoyoshi MISHIMA³, Kenji SHIOJIMA¹
¹University of Fukui, ²SCIOCS, ³Hosei University

D4-11-P04

High Breakdown-Capability Vertical GaN p-n Junction Diodes

Hiroshi OHTA¹, Naomi ASAI¹, Fumimasa HORIKIRI²,
Yoshinobu NARITA², Takehiro YOSHIDA²,
Tomoyoshi MISHIMA¹
¹HOSEI University, ²SCIOCS Co. Ltd

D4-11-P05

Contactless Photoelectrochemical Etching of n-GaN in K₂S₂O₈ solution

Masachika TOGUCHI¹, Kazuki MIWA¹,
Fumimasa HORIKIRI², Noboru FUKUHARA²,
Yoshinobu NARITA², Takehiro YOSHIDA², Taketomo SATO¹
¹Hokkaido University, ²SCIOCS CO., Ltd.

D4-11-P06

Precise Control in Threshold Voltage of AlGaIn/GaN HEMTs by Photoelectrochemical Etching

Yuto KOMATSU, Masachika TOGUCHI, Taketomo SATO
Hokkaido University

D4-11-P07

Effect of Optical and Acoustic Phonons on Optical Properties of Yb₂O₃ and Lu₂O₃ Thin Films

Takaho ASAI¹, Takayuki MAKINO¹, K KAMINAGA²,
Daichi OKA³, Tomoteru FUKUMURA^{2,3}
¹University of Fukui, ²Tohoku University

Cluster E

Magnet and Spintronics

Symposium

- E-1** New Aspects of Understanding Magnetic Materials
- E-2** Spin Conversion Phenomena in Spin Orbit Materials
- E-3** Quantum State in Low Symmetry Environment Probed by Advanced Spin Polarized Quantum Beam

December 12–13, 2019

Symposium E-1

New Aspects of Understanding Magnetic Materials

[Organizers]

Takashi MIYAKE (National Institute of Advanced Industrial Science and Technology)
 Chiharu MITSUMATA (National Institute for Materials Science)
 Leonid POUROVSKII (Ecole Polytechnique)

December 12, 2019

Oral Session 5

Time 14:00–16:00 Room Mont-3

Chairperson Christian ELSÄSSER

E1-12-101 ▶ Invited 14:00–14:30

Magnetic Anisotropy in L1₀-FeNi Magnet: Experiment and Theory

Masaki MIZUGUCHI, Koki TAKANASHI
 Tohoku University

E1-12-002 14:30–14:45

A Brief Review of MnBi-Based Hard Magnetic Materials

Jun CUI¹
¹Critical Materials Institute, Ames Laboratory, ²Materials Science & Engineering, Iowa State University

E1-12-103 ▶ Invited 14:45–15:15

Crystal field, Kondo effect and magnetic anisotropy in perspective rare-earth based hard magnets

Leonid POUROVSKII^{1,2}
¹CPHT, CNRS, Ecole Polytechnique, IP Paris, F-91128 Palaiseau, France, ²Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France

E1-12-004 15:15–15:30

Optimal 4*f*-3*d* Exchange Couplings in Rare-Earth Permanent Magnets

Munehisa MATSUMOTO¹, Takafumi HAWAI^{1,2}, Kanta ONO^{1,2,3}
¹Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK), ²Elements Strategy Initiative Center for Magnetic Materials, National Institute for Materials Science, ³Materials Research by Information Integration Initiative, National Institute for Materials Science

E1-12-005 15:30–15:45

First-principles study of interface magnetism in materials structures of Nd-Fe-B sintered magnets

Asako TERASAWA, Yoshihiro GOHDA
 Tokyo Institute of Technology

E1-12-006 15:45–16:00

Heterogeneous Sm-Co Sintered Magnets With Improved Flexural Strength

BAOZHI CUI
 Ames Laboratory, US Department of Energy

December 13, 2019

Oral Session 7

Time 9:00–11:30 Room Mont-4

Chairperson Leonid POUROVSKII

E1-13-101 ▶ Invited 9:00–9:30

Functional magnetic materials from data-mining and self-organized maps

Olle ERIKSSON^{1,2}
¹Uppsala University, ²Örebro University

E1-13-102 ▶ Invited 9:30–10:00

Screening of rare-earth-lean intermetallic 1-11-X, 1-12-X, and 1-13-X compounds for hard-magnetic applications

Christian ELSÄSSER
 Fraunhofer IWM

E1-13-003 10:00–10:15

Thermodynamic Stability Study of Substitutional Elements in (R,M)(Fe,X)₁₂ Structure using Special Quasirandom Structures

Arkapol SAENGDEEJING, Ying CHEN
 Tohoku University

Short Break

10:15–10:30

E1-13-104 ▶ Invited 10:30–11:00

Ensemble Learning Reveals Similarity Between Rare-earth Transition Metal Binary Alloys

Hieu Chi DAM^{1,2}, Nguyen Duong NGUYEN¹, Viet Cuong NGUYEN³, Hiori KINO², Takashi MIYAKE^{2,4}
¹Japan Advanced Institute of Science and Technology, 1-1 Asahidai, Nomi, Ishikawa 923-1292, Japan, ²National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan, ³HPC Systems Inc., Minato, Tokyo 108-0022, Japan, ⁴CD-FMat, Advanced Institute of Science and Technology, 1-1-1 Umezono, Tsukuba 305-8568, Japan

E1-13-005 11:00–11:15

Can Non-Critical Rare Earths Be Used For Permanent Magnets?

David PARKER
 Oak Ridge National Laboratory

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

E1-13-006 11:15–11:30

Cerium-Based Gap Magnets. Recent Advances In Understanding And Optimization.

Andriy PALASYUK¹, Savannah DOWNING²,
Olena PALASYUK^{1,3}, Tae-Hoon KIM¹, Matthew LYNN¹,
Lin ZHOU¹, Matthew KRAMER^{1,3}, Sergey BUD'KO^{1,2},
Paul CANFIELD^{1,2}

¹Ames Laboratory, ²Department of Physics and Astronomy,
Iowa State University, ³Department of Material Science and
Engineering, Iowa State University

December 13, 2019

Oral Session 8

Time 14:00–16:00 Room Mont-4

Chairperson Olle ERIKSSON

E1-13-107 ▶ Invited 14:00–14:30

Chiral Magnetic Skyrmions For Information Technology

Stefan BLÜGEL¹, Markus HOFFMANN^{1,2},
Bernd ZIMMERMANN^{1,2}, Gideon MÜLLER^{1,2}, Hongying JIA^{1,2}
¹Forschungszentrum Jülich, ²JARA

E1-13-108 ▶ Invited 14:30–15:00

Atomistic Approach to the Nd₂Fe₁₄B magnet

Seiji MIYASHITA^{1,3,6}, Yuta TOGA⁶, Masamichi NISHINO^{2,6},
Taichi HINOKIHARA^{3,6}, Ismail UYSAL^{2,6}, Akimasa SAKUMA⁴,
Takashi MIYAKE⁵, Hisazumi AKAI^{3,6}, Satoshi HIROSAWA⁶

¹The Physical Society of Japan, ²National Institute
for Materials Science(NIMS), ³Institute for Solid State
Physics, The University of Tokyo, ⁴Department of Applied
Physics, Tohoku University, ⁵CD-FMat, National Institute
of Advanced Industrial Science and Technology (AIST),
⁶ESICMM(The Elements Strategy Initiative Center for
Magnetic Materials), NIMS

E1-13-009 15:00–15:15

Temperature dependence of coercivity in Nd₂Fe₁₄B atomistic spin model

Yuta TOGA^{1,6}, Seiji MIYASHITA^{2,3,6}, Akimasa SAKUMA⁴,
Takashi MIYAKE^{5,6}

¹National Institute for Materials Science (NIMS), ²The
Physical Society of Japan, ³Institute for Solid State
Physics, The University of Tokyo, ⁴Department of Applied
Physics, Tohoku University, ⁵National Institute of Advanced
Industrial Science and Technology (AIST), ⁶Elements
Strategy Initiative Center for Magnetic Materials (ESICMM)

E1-13-010 15:15–15:30

Micromagnetic simulation of magnetization reversals and domain wall motions inside permanent magnet

Hiroshi TSUKAHARA¹, Kaoru IWANO¹, Tadashi ISHIKAWA¹,
Chiharu MITSUMATA², Kanta ONO¹

¹High Energy Accelerator Research Organization, ²National
Institute for Materials Science

E1-13-111 ▶ Invited 15:30–16:00

Ginzburg-Landau Type Analysis of Permanent Magnets with Perpendicular Anisotropy

Kaoru IWANO¹, Chiharu MITSUMATA², Hiroshi TSUKAHARA¹,
Kanta ONO¹

¹High Energy Research Organization, ²National Institute of
Materials Science

December 13, 2019

Oral Session 9

Time 16:30–17:30 Room Mont-4

Chairperson Stefan BLÜGEL

E1-13-012 16:30–16:45

A first-principles study on magnetic damping at Fe/MgO(001)

Yoshio MIURA

National Institute for Materials Science

E1-13-013 16:45–17:00

Theoretical Study for Interfacial Magnetic Anisotropy in Magnetic Tunnel Junctions

Keisuke MASUDA, Yoshio MIURA

National Institute for Materials Science (NIMS)

E1-13-014 17:00–17:15

Withdrawal

E1-13-015 17:15–17:30

Study on magnetization dynamics in magnetic wires on LiNbO₃

Shunya SAEGUSA

University of Hyogo

December 12, 2019

Poster Session

Time 16:30–18:00 Room Trade-0

E1-12-P01

First-principles Study on Electric Structure and Magnetic Properties of Yttrium Iron Garnet from Constrained DFT Approach

Hiroki NAKASHIMA, Abdul-Muizz PRADIPTO,
Toru AKIYAMA, Tomonori ITO, Kohji NAKAMURA
Mie University

E1-12-P02

Electric Field Effect on Magnetocrystalline Anisotropy in 3d Transition-metal Thin Films

Thi Phuong Thao NGUYEN

Osaka University

Symposium A
 Symposium B
 Symposium C
 Symposium D
 Symposium E
 Symposium F
 Symposium G
 Symposium H
 Symposium I
 E1-12-P03

Computational materials design of spin-gapless quaternary Heusler alloys

 Fumiaki KURODA¹, Tetsuya FUKUSHIMA^{1,2,3},
 Tamio OGUCHI^{1,2}
¹The Institute of Scientific and Industrial Research, Osaka Univ., ²Center for Spintronics Research Network, Osaka Univ., ³Institute for NanoScience Design, Osaka Univ.

E1-12-P04

Theoretical Sm-Fe-Cu ternary phase diagram for subphase-exploration of SmFe₁₂ permanent magnets

 Sonju KOU¹, Taichi ABE², Yoshihiro GOHDA¹
¹Tokyo Institute of Technology, ²National Institute for Materials Science

E1-12-P05

First-principles based calculation of magnetic properties at finite temperature

Shotaro DOI

National Institute of Advanced Industrial Science and Technology

E1-12-P06

Magnetic properties of Fe-doped CuCrO₂ Electrospun nanofibers

Rattakarn YENSANO

Department of Physics, Faculty of Science, Khon Kaen University

E1-12-P07

Theoretical Prediction of Maximum Curie temperatures of Fe-based Dilute Magnetic Semiconductors by First-principles Calculations

 Tetsuya FUKUSHIMA^{1,2,3}, Hikari SHINYA^{3,4}, Akira MASAGO³,
 Kazunori SATO^{3,5}, Hiroshi KATAYAMA-YOSHIDA⁶
¹Institute for NanoScience Design, Osaka University, ²Center for Spintronics Research Network, Osaka University, ³Research Institute of Electrical Communication, Tohoku University, ⁴Graduate School of Engineering, Osaka University, ⁵Center for Spintronics Research Network, The University of Tokyo

E1-12-P08

Search for Stable Compounds in Y-Fe Binary System: Application of Evolutionary Construction Technique of Formation Energy Convex Hull

 Takahiro ISHIKAWA¹, Takashi MIYAKE^{2,1}
¹ESICMM, National Institute for Materials Science, ²CD-FMat, National Institute of Advanced Industrial Science and Technology

E1-12-P09

Linearly Independent Descriptor Generation Method for Interpretable Modeling

 Hitoshi FUJII^{1,2}, Tetsuya FUKUSHIMA^{3,4}, Tamio OGUCHI^{1,2}
¹National Institute for Materials Science, ²Institute of Scientific and Industrial Research, ³Institute for NanoScience Design, ⁴Institute for Dataability Science

E1-12-P10

Effects of Electron-phonon Scattering on Temperature Dependence of Half-metallicity of Co₂MnSi

Naomi HIRAYAMA, Hisazumi AKAI

The Institute for Solid State Physics, The University of Tokyo

E1-12-P11

Fabrication of L1₀-type FeCo ordered structure using a periodic Ni buffer layer

 Hisaaki ITO¹, Masahiro SAITO¹, Toshio MIYAMACHI², Fumio KOMORI², Tomoyuki KOGANEZAWA³,
 Masaki MIZUGUCHI^{4,5}, Masato KOTSUGI¹
¹Tokyo University of Science, ²The Institute for Solid State Physics, The University of Tokyo, ³Japan Synchrotron Radiation Research Institute (JASRI/SPRING-8), ⁴Institute for Materials Research, Tohoku University, ⁵Center for Spintronics Research Network, Tohoku University

E1-12-P12

Evidence of Non-Joulian Magnetostriction for Fe-Ga and Fe-Al Single Crystal Alloys.

Masaki FUJITA

Tokyo City University

E1-12-P13

First-principles electronic structure calculations of rare-earth nitrides by using quasi-particle self-consistent GW method

 Kazunori SATO^{1,2}, Takao KOTANI³
¹Division of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, ²Center for Spintronics Research Network (CSRN), Osaka University, ³Department of Applied Mathematics and Physics, Tottori University

E1-12-P14

Magnetic Bulk Rashba Effect in Ferroelectric Materials: A First-Principles Study

 Kunihiko YAMAUCHI¹, Paolo BARONE², Silvia PICOZZI²
¹ISIR-SANKEN, Osaka University, ²Consiglio Nazionale delle Ricerche (CNR-SPIN)

E1-12-P15

First-principles calculation of (R, Zr)(Fe, Co, Ti)₁₂ (R = Y, Nd, Sm)

 Taro FUKAZAWA^{1,2}, Yosuke HARASHIMA^{1,2,3},
 Takashi MIYAKE^{1,2}
¹CD-FMat, National Institute of Advanced Industrial Science and Technology, ²ESICMM, National Institute for Materials Science, ³IMaSS, Nagoya University

E1-12-P16

First-principles study of magnetic properties of Nd-Fe alloys in Nd-Fe-B magnets

Yuta AINAI

Tokyo Tech

E1-12-P17**First-Principles Study on Piezoelectricity and Magnetic Stability in Bi(Fe,Co)O₃**

Hiroshi KATSUMOTO, Kunihiko YAMAUCHI, Tamio OGUCHI
Institution of Scientific and Industrial Research, Osaka University

E1-12-P18**Spin wave dispersion of 3d ferromagnets based on QSGW calculations**

Haruki OKUMURA¹, Kazunori SATO¹, Takao KOTANI²
¹Division of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, ²Department of Applied Mathematics and Physics, Tottori University

E1-12-P19**Magnetic polaron and unconventional magneto-transport properties in single crystalline EuBiTe₃ compound**

Won Hyuk SHON¹, Jong-Soo RHYEE¹, Yingshi JIN²,
Sung-Jin KIM²
¹Kyung Hee University, ²Ewha Womans University

December 11, 2019

Symposium E-2

Spin Conversion Phenomena in Spin Orbit Materials

[Organizers]

YoshiChika OTANI (ISSP University of Tokyo)
Akira OIWA (ISIR Osaka University)

December 11, 2019

Oral Session 2

Time 14:00–16:20 Room Miel-5

Chairpersons A. OIWA, T. HIGO

E2-11-I01 ▶ Invited 14:00–14:25

Large time-reversal-odd responses in the topological antiferromagnet Mn_3Sn

Tomoya HIGO^{1,2}, Huiyuan MAN^{1,3}, Muhammad IKHLAS¹, Danru QU^{1,4}, Yoshichika OTANI^{1,2,5}, Satoru NAKATSUJI^{1,2,3,6}
¹ISSP, University of Tokyo, ²JST-CREST, ³Johns Hopkins University, ⁴Institute of Physics, Academia Sinica, ⁵RIKEN-CEMS, ⁶Dept. of Physics, University of Tokyo

E2-11-002 14:25–14:40

Magneto-transport properties in the chiral antiferromagnet Mn_3Sn thin film

Ayuko KOBAYASHI¹, Danru QU^{1,2}, Tomoya HIGO^{1,3}, Satoru NAKATSUJI^{1,3,4,5}, Yoshichika OTANI^{1,3,6}
¹ISSP, University of Tokyo, ²Institute of Physics, Academia Sinica, ³JST-CREST, ⁴Johns Hopkins University, ⁵Dept. of Physics, University of Tokyo, ⁶RIKEN-CEMS

E2-11-003 14:40–14:55

Large Spin Anomalous Hall Effect in $L1_0$ -FePt

Takeshi SEKI^{1,2}, Satoshi IIHAMA³, Tomohiro TANIGUCHI⁴, Koki TAKANASHI^{1,2}
¹Institute for Materials Research, Tohoku University, Japan, ²Center for Spintronics Research Network, Tohoku University, Japan, ³WPI Advanced Institute for Materials Research, Tohoku University, Japan, ⁴AIST, Japan

E2-11-004 14:55–15:10

Observation of Inverse Spin Hall Effect at First-order Magnetic Phase Transition Temperature

Kenta MATSUMOTO¹, Kouta KONDOU^{1,2}, Tomoya HIGO¹, Jamie R. MASSEY³, Rowan C. TEMPLE³, Christopher H. MARROWS³, YoshiChika OTANI^{1,2}
¹ISSP, the University of Tokyo, ²RIKEN-CEMS, ³School of Physics and Astronomy, University of Leeds

E2-11-I05 ▶ Invited 15:10–15:35

Magnetic spin Hall effect in chiral antiferromagnet Mn_3Sn

Kouta KONDOU^{1,2,3}, Motoi KIMATA³, Hua CHEN^{4,5}, Satoshi SUGIMOTO³, Prasanta Kumar MUDULI³, Ikhlas MUHAMMAD³, Takahiro TOMITA^{2,3}, Allan Hugh MACDONALD⁴, Satoru NAKATSUJI^{2,3}, Yoshichika OTANI^{1,2,3}
¹RIKEN, ²CREST, Japan Science and Technology Agency (JST), ³Institute for Solid State Physics, University of Tokyo, ⁴Department of Physics, University of Texas at Austin, ⁵Department of Physics, Colorado State University

E2-11-006 15:35–15:50

Semi-metallic bulk generated spin-orbit torque in disordered topological insulator

Tenghua GAO, Kazuya ANDO
Keio University

E2-11-007 15:50–16:05

Comparison of Spin Hall Angles for Epitaxial and Polycrystalline Platinum Thin Films

Zheng ZHU¹, Tomoya HIGO^{1,2}, Junyeon KIM³, Kenta MATSUMOTO¹, Hironari ISSHIKI¹, Danru QU⁴, Kouta KONDOU³, Satoru NAKATSUJI^{1,2}, Yoshichika OTANI^{1,2,3}
¹Institute for Solid State Physics, The University of Tokyo, ²JST CREST, ³RIKEN-CEMS, ⁴Institute of Physics, Academia Sinica

E2-11-008 16:05–16:20

Spin Hall effect in highly oriented bismuth by using spin-torque ferromagnetic resonance

Masayuki MATSUSHIMA¹, Yuichiro ANDO¹, Ryo OHSHIMA¹, Sergey DUSHENKO¹, Ei SHIGEMATSU¹, Takeshi KAWABE², Teruya SHINJO¹, Shinji MIWA², Masashi SHIRAISHI¹
¹Kyoto University, ²The University of Tokyo

December 11, 2019

Oral Session 3

Time 16:30–18:35 Room Miel-5

Chairpersons K. KONDOU, A. OIWA

E2-11-I09 ▶ Invited 16:30–16:55

Spintronic operations with antiferromagnets

Takahiro MORIYAMA
Kyoto University

E2-11-010 16:55–17:10

Spin currents in nearly-compensated ferrimagnetic insulators

Rafael RAMOS
Advanced Institute for Materials Research, Tohoku University

E2-11-011 17:10–17:25

Conversion between electron spin and phonon angular momentumMasato HAMADA, Shuichi MURAKAMI
Tokyo Institute of Technology

E2-11-012 17:25–17:40

An effective way to control the orbital magnetic momentShengqun SU
IMCE, Kyushu University

E2-11-113 ▶ Invited 17:40–18:05

Optical excitation and detection of ultrafast antiferromagnetic stateTakuya SATOH
Tokyo Institute of Technology

E2-11-014 18:05–18:20

Excitation and propagation dynamics of spin waves observed by phase-resolved spin-wave tomographyYusuke HASHIMOTO
Tohoku University

E2-11-015 18:20–18:35

Ultrafast spin dependent phenomena and opt-magnetic control in ferrimagnetic rear-earth transition metal alloyArata TSUKAMOTO
Nihon University

December 11, 2019

Poster Session**Time** 19:00–20:30 **Room** Trade-0

E2-11-P01

Electrical detection of all-optical magnetization switching in ferrimagnetic GdFeCo alloy by anomalous Hall effectYuichi KASATANI^{1,2}, Hiroki YOSHIKAWA¹, Arata TSUKAMOTO¹
¹Nihon University, ²JSPS Research Fellow

E2-11-P02

ColrMnAl: A potential candidate for spintronics applicationTufan ROY¹, Masahito TSUJIKAWA^{1,2}, Takuro KANEMURA¹, Masafumi SHIRAJI^{1,2,3}¹Research Institute of Electrical Communication, Tohoku University, ²Center for Spintronics Research Network, Tohoku University, ³Center for Science and Innovation in Spintronics (CSIS), Core Research Cluster (CRC), Tohoku University

E2-11-P03

Nonreciprocal spin current conversion from non-uniform charge-current flowGenki OKANO¹, Mamoru MATSUO^{2,3}, Yuichi OHNUMA^{2,3}, Sadamichi MAEKAWA^{3,2}, Yukio NOZAKI^{1,4}¹Department of Physics, Keio University, ²Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences, ³RIKEN CEMS, ⁴Center for Spintronics Research Network, Keio University

E2-11-P04

Magnetic properties of a Co₂FeSi/BaTiO₃ interfacial multiferroic systemShinya YAMADA^{1,2}, Yuki TERAMOTO², Taichi MURATA², Daishi MATSUMI², Kohei KUDO², Tomoyasu TANIYAMA³, Kohei HAMAYA^{1,2}¹Center for Spintronics Research Network, Graduate School of Engineering Science, Osaka University, ²Department of Systems Innovation, Graduate School of Engineering Science, Osaka University, ³Department of Physics, Nagoya University

E2-11-P05

First-principles Calculation of Spin Properties in Two-dimensional Systems Under In-plane Electric FieldsNaoya YAMAGUCHI¹, Fumiyuki ISHII²¹Graduate School of Natural Science and Technology, Kanazawa University, ²Nanomaterials Research Institute, Kanazawa University

E2-11-P06

Optical detection of magnetization dynamics and damping for synthetic antiferromagnetAkira KAMIMAKI^{1,2}, Satoshi IIHAMA^{2,3}, Tomohiro TANIGUCHI⁴, Shigemi MIZUKAMI^{2,3,5}¹Department of Applied Physics, Graduate School of Engineering, Tohoku University, Japan, ²WPI Advanced Institute for Materials Research (AIMR), Tohoku University, Japan, ³Center for Spintronics Research Network (CSRN), Tohoku University, Japan, ⁴National Institute of Advanced Industrial Science and Technology (AIST), Spintronics Research Center, Japan, ⁵Center for Science and Innovation in Spintronics (CSIS), Core Research Cluster (CRC), Tohoku University, Japan

E2-11-P07

Spin dependent transport properties in the magnetic tunnel junctions with a Cr₂O₃ barrier layerTomohiro ICHINOSE¹, Kelvin ELPHICK², Atsufumi HIROHATA², Shigemi MIZUKAMI^{1,3,4}¹WPI-AIMR, Tohoku University, ²Department of Electronic Engineering, University of York, ³CSIS, Tohoku University, ⁴CSRN, Tohoku University

E2-11-P08

Inverse Edelstein effect Induced by magnon-phonon CouplingMingran XU¹, Jorge PUEBLA², Florent AUVRAY¹, Bivas RANA², Kouta KONDOU², Yoshichika OTANI^{1,2}¹Institute for Solid State Physics, University of Tokyo, ²CEMS, RIKEN



E2-11-P09

Electric field control of damping constant

Bivas RANA¹, Collins Ashu AKOSA¹, Gen TATARA¹, YoshiChika OTANI^{1,2}

¹CEMS, RIKEN, ²Institute for Solid State Physics, University of Tokyo

E2-11-P10

Gate control of intra-Landau level transition and observation of spin precession at quantum Hall state

Takase SHIMIZU, Yoshiaki HASHIMOTO, Taketomo NAKAMURA, Akira ENDO, Shingo KATSUMOTO
The institute for solid state physics, the University of Tokyo

E2-11-P11

Spin transport properties in antiferromagnetic L₁2-ordered Mn₃Ir thin films

Hiroyuki IWAKI, Takahiro MORIYAMA, Tetsuya IKEBUCHI, Kento ODA, Yoichi SHIOTA, Teruo ONO
Institute for Chemical Research, Kyoto University

E2-11-P12

Magnon-phonon interaction induced thermal Hall effect in the triangular antiferromagnet

Takuma SAITO
Department of Applied Physics, The University of Tokyo

E2-11-P13

Crystal orientation dependence of the spin current transmission in single crystalline NiO thin films

Tetsuya IKEBUCHI, Takahiro MORIYAMA, Kent ODA, Hiroyuki IWAKI, Teruo ONO
Kyoto University

E2-11-P14

Fabrication and rectifying properties of epitaxial magnetic tunnel junctions with metastable rock-salt ZnO tunnel barrier

Hidekazu SAITO¹, Shintaro KON^{1,2}, Yukiko YASUKAWA², Hiroshi IMAMURA¹, Shinji YUASA¹

¹National Institute of Advanced Industrial Science and Technology, Spintronics Research Center, ²Chiba Institute of Technology

E2-11-P15

Photoinduced Rashba spin-to-charge conversion via an interfacial unoccupied state

Jorge PUEBLA
Center of Emergent Matter Science RIKEN

E2-11-P16

Spin-blockade and Rashba-resonance in a double quantum well diode

Taketomo NAKAMURA, Yoshiaki HASHIMOTO, Shingo KATSUMOTO
The University of Tokyo

E2-11-P17

Spin dynamics in nanostructures probed by quantum dot sensors

Tomohiro OTSUKA¹, Takashi NAKAJIMA², Matthieu R. DELBECQ², Peter STANO², Shinichi AMAHA², Jun YONEDA², Kenta TAKEDA², Gilles ALLISON², Sen LI², Akito NOIRI², Takumi ITO², Daniel LOSS², Arne LUDWIG³, Andreas D. WIECK³, Seigo TARUCHA²

¹Tohoku University, ²RIKEN, ³Ruhr-Universität Bochum

E2-11-P18

Quantum spin transport to self-assembled InGaAs quantum dots through AlGaAs/GaAs superlattice

Satoshi HIURA¹, Junichi TAKAYAMA¹, Takayuki KIBA², Akihiro MURAYAMA¹

¹Hokkaido University, ²Kitami Institute of Technology

E2-11-P19

Detection of optical spin orientation by inverse spin Hall effect in (110)-AlGaAs/GaAs quantum well

Yuji SAKAI¹, Tomohiro NAKAGAWA¹, Julian RITZMANN², Andreas WIECK², Arne LUDWIG², Akira OIWA¹

¹ISIR, Osaka University, ²Ruhr-Universität

December 11–13, 2019

Symposium E-3**Quantum State in Low Symmetry Environment Probed by Advanced Spin Polarized Quantum Beam**

[Organizers]

Koichiro SHIMOMURA (High Energy Accelerator Research Organization)
Wataru HIGEMOTO (Japan Atomic Energy Agency)

December 11, 2019

Oral Session 2

Time 14:00–16:00 Room Trade-2

Chairperson E. TORIAI

E3-11-001

14:00–14:25

Coexistence of Dynamical and Static Component of Molecular Dynamics in Polybutadiene Probed by Muon Spin RelaxationSoshi TAKESHITA¹, Hirohisa OKABE¹, Akihiro KODA¹, Masatoshi HIRAISHI¹, Kenji KOJIMA^{1,2}, Ryosuke KADONO¹, Hideki SETO¹, Tomomi MASUI³, Noboru WAKABAYASHI³¹High Energy Accelerator Research Organization (KEK),
²TRIUMF, ³Sumitomo Rubber Industries, Ltd

E3-11-002

14:25–14:50

 μ SR Study of Glycine, Oligoglycine and N-methylacetamideYoko SUGAWARA^{1,2}, Amba D. PANT³, Takahisa FUJITA², Shigefumi YAMAMURA², Akihiro KODA⁴, Wataru HIGEMOTO⁵, Koichiro SHIMOMURA⁴, Katsuhiko ISHIDA⁶, Eiko TORIKAI⁷, Kanetada NAGAMINE⁴¹Toyota Physical & Chemical Research Institute, ²Kitasato University, ³Ibaraki University, ⁴IMSS, KEK, ⁵Atomic Energy Agency, ⁶RIKEN, ⁷University of Yamanashi

E3-11-003

14:50–15:15

Direct Observation of Electron and Proton Transfers in Enzymatic Reactions by μ SRTamiko KIYOTAN¹, Ichiro TANAKA², Nobuo NIIMURA²¹Showa Pharmaceutical University, ²Ibaraki University

E3-11-004

15:15–15:40

An Application of μ SR in Biology, The Electron Transfer in DNAIsao WATANABE¹, Harison ROZAK^{1,2,3}, Wan Nurfadhilah ZAHARIM^{2,3}, Issei MIYAZAKI⁴, Nur Eliana ISMAIL², Siti Nuramira ABU BAKAR², Daruliza KERNAIN², Razip SAMIAN², Koichi ICHIMURA⁴, Mohamed Ismail MOHAMED-IBRAHIM^{2,3}, Shukri SULAIMAN^{2,3}¹RIKEN, ²Universiti Sains Malaysia, ³USM-RIKEN International Center for Ageing Science, ⁴Hokkaido University

E3-11-005

15:40–16:00

First Principles Theory of Hyperfine Interactions in Guanine NucleobaseIsao WATANABE¹, Wan Nurfadhilah ZAHARIM^{2,3}, Shukri SULAIMAN^{2,3}, Siti Nuramira ABU BAKAR^{2,3}, Nur Eliana ISMAIL^{2,3}, Harison ROZAK^{1,2,3}¹RIKEN, ²Universiti Sains Malaysia, ³USM-RIKEN International Center for Ageing Science, ⁴Hokkaido University

December 11, 2019

Oral Session 3

Time 16:30–18:35 Room Trade-2

Chairperson K. SHIMOMURA

E3-11-006

► Invited

16:30–16:55

Photoexcited μ SR Experiments at the ISIS Pulsed Neutron and Muon SourceKoji YOKOYAMA, James S. LORD

ISIS, STFC Rutherford Appleton Laboratory, Didcot, OX11 0QX, United Kingdom

E3-11-007

16:55–17:20

Progress and prospects of new DC muon source and muon analysis at MuSIC-RCNP, Osaka UniversityDai TOMONO

Osaka University

E3-11-008

17:20–17:45

Generation of Ultra Cold Muonium from Silicon into VacuumAmba Datt PANT^{1,2}, Hiromi IINUMA¹, Katsuhiko ISHIDA³, Chiori OGHANE¹, Moe SUGITA¹, Koichiro SHIMOMURA²¹Institute of Quantum Beam Science, Ibaraki University, Mito, 310-8512, Japan, ²Institute of Materials Structure Science, KEK, Tsukuba, 305-0801, Japan, ³Advanced Meson Science Laboratory, RIKEN, Wako, 351-0198, Japan

E3-11-009

17:45–18:10

Muon Spin Resonance Experiment in the High Magnetic Field at J-PARCShoichiro NISHIMURA

High Energy Accelerator Research Organization

E3-11-010

18:10–18:35

Negative-Muon Decelerator for Material ScienceChihiro OHMORI

KEK

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 12, 2019

Oral Session 4
Time 9:00–11:30 **Room** Trade-3

Chairperson T. ADACHI

E3-12-001 9:00–9:25

Transformation of interstitial proton into substitutional hydride in reduced SrTiO₃ simulated with positively charged muons

 Takashi U. ITO^{1,2}, Wataru HIGEMOTO^{1,2,3}, Akihiro KODA^{2,4}, Koichiro SHIMOMURA^{2,4}
¹Advanced Science Research Center, Japan Atomic Energy Agency, ²Muon Science Section, MLF Division, J-PARC Center, ³Department of Physics, Tokyo Institute of Technology, ⁴Institute of Materials Structure Science, High Energy Accelerator Research Organization

E3-12-002 9:25–9:50

Local Electronic Structure of Interstitial Hydrogen in Iron Disulfide

Ryosuke KADONO

Institute of Materials Structure Science, KEK

E3-12-003 9:50–10:15

Electronic Structure of Interstitial Hydrogen in Electride LaScSi Probed by Muon Spin Rotation Technique

 Masatoshi HIRAISHI¹, Kenji KOJIMA^{1,2}, Hirotaka OKABE¹, Soshi TAKESHITA¹, Akihiro KODA^{1,2}, Ryosuke KADONO^{1,2}, Jiazhen WU³, Hideo HOSONO^{3,4}
¹KEK IMSS, ²SOKENDAI, ³MSL, Tokyo Tech., ⁴MCES, Tokyo Tech.

E3-12-104 ▶ Invited 10:15–10:40

μSR Approach To The Understanding Of Hydrogen Embrittlement In Steels

Nobuhiko NISHIDA

JAEA

E3-12-005 10:40–11:05

Muon Spin Relaxation in a Hydrogen Charged Al-0.2%Cu Alloy

 Katsuhiko NISHIMURA¹, Kenji MATSUDA¹, Takahiro NAMIKI¹, Seungwon LEE¹, Wataru HIGEMOTO², Yasuhiro MIYAKA³, Hiroyuki TODA⁴, Kazuyuki SHIMIZU⁴
¹University of Toyama, ²Japan Atomic Energy Agency, ³High Energy Accelerator Research Organization, ⁴Kyushu University

E3-12-006 11:05–11:30

Hydrogen Absorption-Desorption Process in Palladium Studied by Muon Spectroscopy

 Mototsugu MIHARA¹, Hideki ARAKI², Koichiro SHIMOMURA³, Wataru HIGEMOTO⁴, Masataka MIZUNO², Kazuki SUGITA², Yuki TANAKA², Yuta KITAYAMA², Dai TOMONO⁵, Eiko TORIKAI⁶, Wataru SATO⁷, Kanji OHKUBO², Ryoma MURAKAMI², Naoki MATSUOKA², Isao WATANABE⁸, Teiichiro MATSUZAKI⁸, Ryosuke KADONO³
¹Department of Physics, Osaka University, ²Division of Materials and Manufacturing Science, Osaka University, ³Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK), ⁴Advanced Science Research Center, Japan Atomic Energy Agency (JAEA), ⁵Research Center for Nuclear Physics (RCNP), Osaka University, ⁶University of Yamanashi, ⁷Institute of Science and Engineering, Kanazawa University, ⁸RIKEN Nishina Center for Accelerator-Based Science

December 12, 2019

Oral Session 5
Time 14:00–16:05 **Room** Trade-3

Chairperson W. HIGEMOTO

E3-12-007 14:00–14:25

Development of Ultra slow muon microscope to probe near surface and buried interface in materials and life science

 Eiko TORIKAI^{1,2}, Yasuhiro MIYAKE^{2,3}, Ryosuke KADONO^{2,3}, Masahiko IWASAKI⁴
¹University of Yamanashi, ²High Energy Accelerator Research Organization, ³J-PARC Center, ⁴RIKEN

E3-12-008 14:25–14:50

Advanced Muon Spin Spectroscopy for Sustainable Society

 Jun SUGIYAMA^{1,2,3}, Wataru HIGEMOTO², Koichiro SHIMOMURA³
¹CROSS-Tokai Neutron Science and Technology Center, ²Advanced Science Research Center, Japan Atomic Energy Agency, ³High Energy Accelerator Research Organization (KEK)

E3-12-009 14:50–15:15

Negative muon spin rotation with low-density gas target under transverse magnetic field

 Sohtaro KANDA, Katsuhiko ISHIDA
RIKEN

E3-12-010 15:15–15:40

Polarized neutron inelastic scattering technique ~powerful probe for solid state physics~

 Takatsugu MASUDA
University of Tokyo

E3-12-011 15:40–16:05
Spin-Polarized ^3He Gas for Polarized Neutron Scattering Measurements
 Takashi INO
 KEK

December 12, 2019

Oral Session 6

Time 16:30–18:55 Room Trade-3

Chairperson R. KADONO

E3-12-012 16:30–16:55
Anisotropy of spontaneous magnetic field in chiral superconductor
 Wataru HIGEMOTO¹, Takeshi OKAZAWA^{1,2}, Yuto ODA^{1,2}, Itsuku MIYAZAKI², Takashi U ITO¹, Yoshiyuki YOSHIDA³
¹Advanced Science Research Center, Japan Atomic Energy Agency, ²Department of Physics, Tokyo Institute of Technology, ³National Institute of Advanced Industrial Science and Technology

E3-12-113 ▶ Invited 16:55–17:20
Spin Fluctuations in High-Temperature Superconductors Probed by Muon
 Tadashi ADACHI
 Sophia University

E3-12-014 17:20–17:45
Magnetotransport and Superconductivity in Spin Momentum–Locked Surface State of Ion-Gated SrTiO_3
 Tsutomu NOJIMA¹, Takumi OUCHI¹, Sunao SHIMIZU^{2,3}, Yoshihiro IWASA^{3,4}
¹Institute for Materials Research, Tohoku University, ²Central Research Institute of Electric Power Industry, ³RIKEN Center for Emergent Matter Science, ⁴Quantum Phase Electronics Center and Department of Applied Physics, University of Tokyo

E3-12-015 17:45–18:10
Magnetism in T*-Type $\text{La}_{1-x/2}\text{Eu}_{1-x/2}\text{Sr}_x\text{CuO}_4$ Studied by μSR Measurement
 Masaki FUJITA¹, Shun ASANO², Kota KUDO², Motofumi TAKAHAMA², Isao WATANABE³, Akihiro KODA⁴, Ryosuke KADONO⁴
¹Institute for Materials Research, Tohoku University, ²Department of Physics, Tohoku University, ³Advanced Meson Science Laboratory, The Institute of Physical and Chemical Research, ⁴Institute of Materials Structure Science, High Energy Accelerator Research Organization

E3-12-016 18:10–18:35
Superconducting Characteristics of MgO/MgB_2 Nanocomposites with a Self-Similar Fractal-Like Structure
 Takashi UCHINO¹, Yusuke SETO¹, Takahiro SAKURAI¹, Hitoshi OHTA¹, Yoshifumi SAKAGUCHI², Kazuki OHISHI², Akihiro KODA³
¹Kobe University, ²CROSS, ³KEK

E3-12-017 18:35–18:55
A Possible Weak Magnetism in Overdoped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ Nanoparticles
 Suci WINARSIH^{1,2,3}, Faisal BUDIMAN^{4,5}, Hirofumi TANAKA⁴, Tadashi ADACHI⁶, Takayuki GOTO⁶, Akihiro KODA⁷, Bambang SOEGLJONO², Budhy KURNIAWAN², Isao WATANABE^{1,2,3}
¹RIKEN, ²Universitas Indonesia, ³Hokkaido University, ⁴Kyushu Institute of Technology, ⁵Telkom University, ⁶Sophia University, ⁷High Energy Accelerator Research Organization (KEK)

December 13, 2019

Oral Session 7

Time 9:00–11:45 Room Trade-1

Chairperson I. WATANABE

E3-13-001 9:00–9:25
Interplay of Magnetic, Electronic and Elastic Degrees of Freedom in Chiral Materials
 Junichiro KISHINE
 The Open University of Japan

E3-13-002 9:25–9:50
Search for Odd-Parity Augmented Multipoles and Cross-Correlation Phenomena in Antiferromagnetic Metals
 Hiroshi AMITSUKA
 Hokkaido University

E3-13-003 9:50–10:15
Strong Enhancement of Spin-orbit Interaction in Alkali Metal Nanoclusters Incorporated into Zeolite A
 Takehito NAKANO
 Ibaraki University

E3-13-004 10:15–10:40
Successive Change of the Motion in Na-loaded Low Silica-X Zeolite According to Loading Density of External Na Atom - An NMR Study -
 Mutsuo IGARASHI¹, Peter JEGLIC², Takehito NAKANO³, Denis ARCON^{2,4}
¹National Institute of Technology, Gunma College, Japan, ²Jozef Stefan Institute, Slovenia, ³Institute of Quantum Beam Science, Graduate School of Science and Engineering, Ibaraki University, Japan, ⁴Faculty of Mathematics and Physics, University of Ljubljana, Slovenia

E3-13-005 10:40–11:05
Magnetic state of $\beta\text{-MnO}_2$ probed by muon spin spectroscopy
 Hirotaka OKABE¹, R. Kadono¹, M. Hiraishi¹, A. Koda¹, S. Takeshita¹, K. M. Kojima², I. Yamauchi³, H. Sato⁴
¹High Energy Accelerator Research Organization (KEK), ²TRIMF, ³Saga University, ⁴Chuo University

E3-13-006

11:05–11:25

Hole Doping Effect on Magnetic Ordering and Spin Dynamic of $(\text{Eu}_{1-x}\text{Ca}_x)_2\text{Ir}_2\text{O}_7$ Studied by μSR

Utami WIDYAI SWARI^{1,2,3}, Julia ANGEL^{1,3}, Hironori NOMURA⁴, Tomoya TANIGUCHI⁴, Kazuyuki MATSUHIRA⁴, Akihiro KODA⁵, Budhy KURNIAWAN², Isao WATANABE^{1,2,3}

¹Meson Science Laboratory, RIKEN Nishina Center, Wako, Saitama, 351-0198, Japan, ²Department of Physics, Faculty of Mathematics and Natural Sciences, Universitas Indonesia, Depok, 16424, Indonesia, ³Department of Condensed Matter Physics, Hokkaido University, Sapporo, 060-0808, Japan, ⁴Faculty of Engineering, Kyushu Institute of Technology, Kitakyushu, 804-8550, Japan, ⁵Muon Science Laboratory, Institute of Materials and Structural Science, High Energy Accelerator Research Organization (KEK), Tokai, Ibaraki, 319-1106, Japan

E3-13-007

11:25–11:45

The admixture of an s-wave component into d-wave superconducting gap symmetry in organic superconductor λ -(BETS) $_2$ GaCl $_4$ studied by μSR

DITA PUSPITA SARI¹, Retno ASIH^{2,3}, Koichi HIRAKI⁴, Takehito NAKANO³, Yasuo NOZUE³, Adrian HILLIER⁵, Yasuyuki ISHII¹, Isao WATANABE^{2,3}

¹Shibaura Institute of Technology, ²Meson Science Laboratory RIKEN, ³Osaka University, ⁴Fukushima Medical University, ⁵ISIS STFC Rutherford Appleton Laboratory

December 13, 2019

Poster Session

Time 14:00–15:30 **Room** Trade-0

E3-13-P01

Neutron Spin Prism Method with High Energy Neutrons at J-PARC

Masaki FUJITA

Institute for Materials Research, Tohoku University

E3-13-P02

Investigation of hydrogen states in semiconducting BaSi $_2$ by muon spin rotation

Takashi SUEMASU¹, Zhihao XU¹, Takuma SATO^{1,2}, Jumpei NAKAMURA³, Akiho KODA^{3,4}, Koichiro SHIMOMURA^{3,4}

¹University of Tsukuba, ²University Grenoble Alpes, ³KEK, ⁴The Graduate University for Advanced Studies

E3-13-P03

 μSR study of the Long-range Ordered State in Organic Antiferromagnet λ -(BEDT-STF) $_2$ FeCl $_4$

DITA PUSPITA SARI¹, Takaaki MINAMIDATE³, Noriaki MATSUNAGA⁴, Atsushi KAWAMOTO⁴, Isao WATANABE², Yasuyuki ISHII¹

¹Shibaura Institute of Technology, ²Meson Science Laboratory RIKEN, ³Condensed Molecular Material Laboratory RIKEN, ⁴Hokkaido University

E3-13-P04

Observation of Hole Localization on Apical Oxygen in Sr $_2$ IrO $_4$ via Oxygen Spin Measured by μSR

Masanori MIYAZAKI¹, Mizuki ISHIHARA¹, Takumi KINOSHITA¹, Yuya NISHIYAMA¹, Hiroshi ISODA¹, Masatoshi HIRAIISHI², Hirotaka OKABE², Kenji M. KOJIMA³, Akihiro KODA², Ryosuke KADONO², Shuji EBISU¹

¹Muroran Institute of Technology, ²High Energy Accelerator Research organization, ³TRIUMF

E3-13-P05

The Effects of Split Valence Basis Sets on Muon Hyperfine Interaction in Guanine Nucleobase and Guanine Nucleotide Structures

WAN NURFADHILAH ZAHARIM^{1,2}, SHUKRI SULAIMAN¹, SITI NUR AFIFI AHMAD¹, SITI NURAMIRA ABU BAKAR¹, NUR ELIANA ISMAIL¹, HARISON ROZAK^{1,2}, ISAO WATANABE^{1,2,3}

¹UNIVERSITI SAINS MALAYSIA, ²RIKEN NISHINA CENTER, ³HOKKAIDO UNIVERSITY

E3-13-P06

Density Functional Theory Investigation of Muon Hyperfine Interactions in Au $_{25}$ Sr $_{18}$ Nanocluster

WAN NURFADHILAH ZAHARIM^{1,2}, SITI NUR AFIFI AHMAD¹, SHUKRI SULAIMAN¹, DANG FATIHAH HASAN BASERI¹, NOR ZAKIAH YAHAYA¹, HASNI ARSAD¹, LEE SIN ANG³, ISAO WATANABE^{2,4}

¹UNIVERSITI SAINS MALAYSIA, ²RIKEN NISHINA CENTER, ³UNIVERSITI TEKNOLOGI MARA, ⁴HOKKAIDO UNIVERSITY

E3-13-P07

Magnetic Phase Diagram of $(\text{Y}_{0.95-x}\text{Cu}_{0.05}\text{Ca}_x)_2\text{Ir}_2\text{O}_7$ Revealed by μSR

Julia ANGEL^{1,2}, Utami WIDYAI SWARI^{1,2,3}, Hironori NOMURA⁴, Tomoya TANIGUCHI⁴, Kazuyuki MATSUHIRA⁴, Isao WATANABE^{1,2,3}

¹Meson Science Laboratory, RIKEN Nishina Center, ²Department of Condensed Matter Physics, Hokkaido University, ³Department of Physics, Faculty of Mathematics and Natural Sciences, Universitas Indonesia, ⁴Faculty of Engineering, Kyushu Institute of Technology

E3-13-P08

DFT and μSR Studies on YBa $_2$ Cu $_3$ O $_6$ and La $_2$ CuO $_4$

Irwan RAMLI^{1,2}, Muhammad Redo RAMADHAN^{1,2,3}, Suci WINARSIH^{1,2,3}, Mohamed Ismail MOHAMED IBRAHIM^{4,5}, Shukri SULAIMAN^{4,5}, Isao WATANABE^{1,2,3,4,5}

¹Meson Science Laboratory, RIKEN Nishina Center, ²Department of Condensed Matter Physics, Graduate School of Science, Hokkaido University, ³Department of Physics, Faculty of Mathematics and Natural Sciences (FMIPA), Universitas Indonesia, ⁴Computational Chemistry and Physics Laboratory, School of Distance Education, Universiti Sains Malaysia, ⁵USM-RIKEN International Center for Ageing Science, School of Distance Education, Universiti Sains Malaysia

E3-13-P09

Shallow donor Hydrogen in TiO $_2$ studied by μSR

Koichiro SHIMOMURA, Ryosuke KADONO, Hua LI KEK IMSS

Cluster F

Energy

Symposium

- F-1** Battery Materials for Sustainability
- F-2** Catalysis and Catalyst Materials for Energy and Environment
- F-3** Advancements in Thermoelectric Materials and Applications
- F-4** Synchrotron X-ray Probes for Mesoscale Materials Science

December 12–13, 2019

Symposium F-1

Battery Materials for Sustainability

[Organizers]

Atsuo YAMADA (The University of Tokyo)
 Shinichi KOMABA (Tokyo University of Science)
 Naoaki YABUUCHI (Yokohama National University)
 Yong-Sheng HU (Chinese Academy of Science)
 Shirley MENG (University of California, San Diego)
 Rosa PALACIN (ICMAB-CSIC)
 Koji OHTA (Kyoto University)

December 12, 2019

Oral Session 4

Time 9:00–11:30 Room Work-5

Chairpersons Atsuo YAMADA, Alexis GRIMAUD,
 Shirley MENG, Patrik JOHANSSON

Opening Talk

Atsuo Yamada

9:00–9:10

F1-12-I01 ▶ Invited 9:10–9:35

How the water solvation structure affects its reduction for the development of aqueous electrolytes for Li-ion batteries

Alexis GRIMAUD

Collège de France, CNRS

F1-12-I02 ▶ Invited 9:35–10:00

Understanding Interfacial Electrochemistry on Highly Oriented Pyrolytic Graphite (HOPG) with Water-In-Salt Electrolyte

Hye Ryung BYON

Korea Advanced Institute of Science and Technology

F1-12-I03 ▶ Invited 10:00–10:25

Robust Prussian Blue Cathodes for Potassium Aqueous Battery with Ultralong Cycle Life and High Power Capability

Yaxiang LU

Institute of Physics, Chinese Academy of Sciences

Break

10:25–10:40

F1-12-I04 ▶ Invited 10:40–11:05

Complex Ionic Liquids & Liquid Ionic Complexes

Patrik JOHANSSON^{1,2}, Piotr JANKOWSKI^{1,2,3}, Gustav ÅVALL¹

¹Chalmers University of Technology, ²Alistore-European Research Institute, ³Warsaw University of Technology

F1-12-I05 ▶ Invited 11:05–11:30

Rational Design of BIAN Based Binder/Additive for Li Ion Secondary Batteries

Noriyoshi MATSUMI, Sai Gourang PATNAIK,

Raman VEDARAJAN

Japan Advanced Institute of Science and Technology

December 12, 2019

Oral Session 5

Time 14:00–16:05 Room Work-5

Chairpersons Shinichi KOMABA, Seung-Taek MYUNG

F1-12-I06 ▶ Invited 14:00–14:25

Phase and Structural Evolution of Layered Positive Electrodes

Neeraj SHARMA

UNSW

F1-12-I07 ▶ Invited 14:25–14:50

Stable Cycling Performance of Manganese-based Cathode Materials for Rechargeable Sodium Batteries

Seung-Taek MYUNG

Sejong University

F1-12-I08 ▶ Invited 14:50–15:15

Novel Phosphates and Fluoride-Phosphates Cathode Materials for Me-ion Batteries

Evgeny ANTIPOV^{1,2}

¹Lomonosov Moscow State University, ²Skolkovo Institute of Science and Technology

F1-12-I09 ▶ Invited 15:15–15:40

Organic Electrodes-based Rechargeable Batteries

Yonggang WANG

Fudan University

F1-12-I10 ▶ Invited 15:40–16:05

Operando X-ray Characterization of Multi-Scale Kinetic Limitations in Battery Electrodes

Karena CHAPMAN

Stony Brook University

December 13, 2019

Oral Session 7

Time 9:00–11:20 Room Work-5

Chairpersons Naoaki YABUUCHI,
 Monste CASAS-CABANAS,
 Yong-Sheng HU, Zheng CHEN

F1-13-I01 ▶ Invited 9:00–9:25

Design of Li and Na fast ion conductors using high-throughput bond-valence calculations

Montse CASAS-CABANAS

CIC energiGUNE

F1-13-I02 ▶ Invited 9:25–9:50

Lithium Metal and the Solid Electrolyte Interphase; past, present and future

Adam BEST
CSIRO Manufacturing

F1-13-I03 ▶ Invited 9:50–10:15

Withdrawal

[Break
10:15–10:30]

F1-13-I04 ▶ Invited 10:30–10:55

Fundamental Processes and Design Strategies for Alkali Metal–Oxygen Batteries

Yi-Chun LU, Yu WANG
The Chinese University of Hong Kong

F1-13-I05 ▶ Invited 10:55–11:20

Leveraging Reversible Chemistry for Materials Sustainability in Energy Storage

Zheng CHEN
University of California San Diego

December 13, 2019

Poster Session

Time 14:00–15:30 Room Trade-0

F1-13-P01

Cation-disordered rocksalt oxides/oxyfluorides for high-energy rechargeable Li/Na batteries

Naoaki YABUUCHI
Yokohama National University

F1-13-P02

Appearance, manipulation, and visualization of lithium-ion conduction in a La–Li–Co–O band insulator

Tsuyoshi TAKAMI¹, Yoshiyuki MORITA¹, Masao YONEMURA², Yoshihisa ISHIKAWA², Shingo TANAKA³, Masahiro MORI³, Toshiharu FUKUNAGA¹, Eiichiro MATSUBARA¹
¹Kyoto University, ²High Energy Accelerator Research Organization, ³National Institute of Advanced Industrial Science and Technology

F1-13-P03

Assessing electrolyte-improved FeF₃ batteries: A universal description characterized by Fe nanoparticles

Tsuyoshi TAKAMI¹, Keitaro MATSUI², Hiroshi SENOH², Noboru TAGUCHI², Masahiro SHIKANO², Hikari SAKAEBE², Toshiharu FUKUNAGA¹
¹Kyoto University, ²National Institute of Advanced Industrial Science and Technology

F1-13-P04

Fabrication of Self-standing Three-Dimensional Porous TiO₂-Si Nano-scaffolds for High Volumetric Capacity Lithium Ion Microbatteries

Wen-Yin KO
National Chung-Hsing University

F1-13-P05

Sensitized “Thermal” Cell

Sachiko MATSUSHITA
Tokyo Institute of Technology

F1-13-P06

A Novel Cathode Material Na₂V₃O₇ for Sodium-Ion Batteries by High-throughput Search

Masanobu NAKAYAMA^{1,2,3}, Naoto TANIBATA^{1,2}, Hayami TAKEDA^{1,2}
¹Nagoya Institute of Technology, ²ESICB, Kyoto University, ³Mi2i, National Institute for Materials Science

F1-13-P07

Computational study of redox process and formation of defects in NaMnO₂ cathode material of Na-ion battery

Maxim SHISHKIN, Hirofumi SATO
ESICB, Kyoto University

F1-13-P08

Ion Conduction Mechanism in Highly Concentrated Sulfolane-Based Electrolytes for Sodium-Ion Batteries

Kaoru DOKKO^{1,2}, Yukihiro OKAMOTO¹, Kazuhide UENO¹, Masayoshi WATANABE¹
¹Yokohama National University, ²Kyoto University

F1-13-P09

Cathode properties of amorphous xNaF-FeSO₄ Systems (1 ≤ x ≤ 2) for sodium ion batteries

Ayuko KITAJOU^{1,4}, Hiroyoshi MOMIDA^{2,4}, Takahiro YAMASHITA³, Tamimo OGUCHI^{2,4}, Shigeto OKADA^{3,4}
¹Yamaguchi University, ²Osaka University, ³Kyushu University, ⁴ESICB, Kyoto University

F1-13-P10

Preparation And Characterization Of a Lithium Ion Conductor Cubic-Li₂FeCl₄

Masashi KATO¹, Koki NAKANO¹, Hayami TAKEDA^{1,2}, Naoto TANIBATA^{1,2}, Masanobu NAKAYAMA^{1,2,3}
¹Nagoya Institute of Technology, ²Kyoto University ESICB, ³National Institute for Materials Science Mi2i & GREEN

F1-13-P11

First-Principles Calculations of X-Ray Absorption Spectra in NaFeSO₄F Cathode for Exploring Na-Ion Battery Reactions

Hiroyoshi MOMIDA^{1,2}, Ayuko KITAJOU^{3,2}, Shigeto OKADA^{4,2}, Tamio OGUCHI^{1,2}
¹Osaka University, ²Kyoto University, ³Yamaguchi University, ⁴Kyushu University

F1-13-P12

A Computational Study on Diffusion of Divalent Ions in Spinel-type Cathodes Materials for Mg Ion Batteries

Taruto ATSUMI¹, Kohei SHIMOKAWA⁴, Maho HARADA¹, Masanobu NAKAYAMA^{1,2,3}, Tetsu ICHITSUBO⁴

¹Nagoya Institute of Technology, ²Kyoto University ESICB, ³MaDiS/CMI2, NIMS, ⁴Tohoku University

F1-13-P13

Electrochemical Properties and Local Structure of NaClO₄ Aqueous Electrolyte for Na-ion Batteries

Maho YAMASHITA¹, Ryo SAKAMOTO², Nobuko YOSHIMOTO¹, Kenta FUJII¹, Ayuko KITAJOU^{1,3}

¹Yamaguchi University, ²Kyushu University, ³ESICB, Kyoto University

F1-13-P14

One-Dimensional Nanoparticles as Anode Materials for LIBs

Mai Thanh NGUYEN¹, Tetsu YONEZAWA¹, Lyn Marie De JUAN-CORPUZ²

¹Hokkaido University, ²Chulalongkorn University

F1-13-P15

Predicting Transport Properties of Ionic Liquids by Using Molecular Dynamics Simulation with DFT-based Force Field

Yoshiki ISHII¹, Nobuyuki MATUBAYASI^{1,2}

¹Osaka University, ²Kyoto University

F1-13-P16

Effect of Thermal Annealing on Chemical Composition and Phase Transition of LiCoO₂ Powders

Awadol KHEJONRAK, Saroj RUJIRAWAT

Suranaree University of Technology

F1-13-P17

Microscopic mechanism of diffusion processes in dilute electrolyte solutions for sodium-ion batteries

Junichi ONO¹, Chien-Pin CHOU¹, Hiromi NAKAI^{1,2,3}

¹Waseda Research Institute for Science and Engineering (WISE), Waseda University, ²Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University, ³Elements Strategy Initiative for Catalysts & Batteries (ESICB), Kyoto University

F1-13-P18

Microscopic Mechanism of SEI Layer Formation in Highly Concentrated Electrolytes Based on the Nonflammable Trimethyl Phosphate Solvent

Amine BOUIBES¹, Norio TAKENAKA^{1,2}, Soumen SAHA^{1,2}, Masataka NAGAOKA^{1,2}

¹Nagoya University, ²ESICB, Kyoto University

F1-13-P19

Reversible Sodium Metal Electrodes: Is Fluorine an Essential Interphasial Component?

Kyosuke DOI¹, Yuki YAMADA^{1,2}, Masaki OKOSHI^{2,3}, Junichi ONO⁴, Chien-Pin CHOU⁴, Hiromi NAKAI^{2,3,4}, Atsuo YAMADA^{1,2}

¹Department of Chemical System Engineering, The University of Tokyo, ²Elements Strategy Initiative for Catalysts & Batteries (ESICB), Kyoto University, ³Department of Chemistry and Biochemistry, Waseda University, ⁴Waseda Research Institute for Science and Engineering (WISE), Waseda University

F1-13-P20

N-Ethyl-N-propylpyrrolidinium Bis(fluorosulfonyl)amide Ionic Liquid Electrolytes with High Na Molar Fraction for Sodium Secondary Batteries

Huan YANG, Jingkwang HWANG, Kazuhiko MATSUMOTO, Rika HAGIWARA, Yushen WANG

Kyoto University

F1-13-P21

A Sulfur-doped Black Phosphorus-TiO₂ Composite as High-Performance Anode Material for Sodium-Ion Storage

Haimei LIU

Shanghai University of Electric Power

F1-13-P22

Battery Performance and Reaction Mechanism in Tin-compounds as Negative Electrode: First-Principles Calculations

Hiroki KOTAKA¹, Hiroyoshi MOMIDA^{1,2}, Tamio OGUCHI^{1,2}

¹Elements Strategy Initiative for Catalysts and Batteries, Kyoto University, ²Scientific and Industrial Research, Osaka University

F1-13-P23

HPO₃²⁻ as Building Unit for Sodium-Ion Battery Cathodes: Na₂Fe(HPO₃)₂

Zihan MA¹, Laura LANDER¹, Masashi OKUBO^{1,2}, Atsuo YAMADA^{1,2}

¹The University of Tokyo, ²Kyoto University, ESICB

F1-13-P24

Microscopic Structure of Electrode/electrolyte Interface Probed by Molecular Simulation and Sum Frequency Generation Spectroscopy

Lin WANG^{1,2}, Satoshi NIHONYANAGI^{3,4}, Ken-ichi INOUE¹, Kei NISHIKAWA⁵, Akihiro MORITA^{1,2}, Shen YE^{1,2}, Tahei TAHARA^{3,4}

¹Department of Chemistry, Graduate School of Science, Tohoku University, ²Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, ³Molecular Spectroscopy Laboratory, RIKEN, ⁴Ultrafast Spectroscopy Research Team, RIKEN Center for Advanced Photonics (RAP), RIKEN, ⁵Rechargeable Battery Materials Group, Center for Green Research on Energy and Environmental Materials, National Institute for Material Sciences

F1-13-P25

Aqueous Alkali Metal-Ion Battery with Naphthalene Tetracarboxylic Diimide-Based Metal-Organic Framework

Kosuke NAKAMOTO¹, Junwen BAI², Liwei ZHAO¹, Ryo SAKAMOTO², Masato ITO¹, Shigeto OKADA¹, Eiji YAMAMOTO³, Haruno MURAYAMA³, Makoto TOKUNAGA³

¹Institute for Materials Chemistry and Engineering, Kyushu University, ²Interdisciplinary Graduate School of Engineering Sciences, Kyushu University, ³Department of Chemistry, Kyushu University

F1-13-P26

Molecular simulations for polymer binder of sodium ion batteries

Hitoshi WASHIZU^{1,2}

¹University of Hyogo, ²Kyoto University

F1-13-P27

Post Lithium-Ion Batteries; Theoretical Characterization of Phosphorous and Tin for Potassium-ion Anodes

Koichi YAMASHITA

Kyoto University

F1-13-P28

Soft X-ray Li-K and Si-Li_{2,3} Emission from Lithium Silicides in Lithium-Ion Batteries Anode

Andrey LYALIN^{1,2}, Vladimir KUZNETSOV³, Akira NAKAYAMA⁴, Igor ABARENKOV³, Ilya TUPITSIN³, Igor GABIS³, Kohei UOSAKI², Tetsuya TAKETSUGU⁵

¹Institute for Chemical Reaction Design and Discovery (ICReDD), Hokkaido University, ²National Institute for Materials Science (NIMS), ³Faculty of Physics, St. Petersburg State University, ⁴Department of Chemical System Engineering, University of Tokyo, ⁵Department of Chemistry, Hokkaido University

F1-13-P29

A Promising Layer Cathode Material for Sodium Ion Batteries: A First Principles Investigation

Huu Duc LUONG

Osaka University

F1-13-P30

Structural and Electrochemical Properties of Nonflammable Solvent-Based Concentrated Electrolytes for Lithium-Ion Batteries

Saki SAWAYAMA, Hideyuki MIMURA, Masayuki MORITA, Kenta FUJII

Yamaguchi University

F1-13-P31

Electrochemical simulation based on the ESM-RISM formalism: a theory and its applications

Yasunobu ANDO^{1,2}, Minoru OTANI^{1,2}

¹CD-FMat, AIST, ²ESICB, Kyoto University

F1-13-P32

Microscope Mechanism of Li-ion Transport at Interfaces between LiCoO₂ Cathode and Sulfide Electrolyte in All-Solid-State Battery via DFT-CALYPSO Method

Bo GAO¹, Randy JALEM¹, Yanming MA², Yoshitaka TATEYAMA¹

¹National Institute for Materials Science, ²Jilin University

F1-13-P33

Electrochemical Sodium-ion Intercalation Behavior into Graphite-Based Electrode

Yasuyuki KONDO¹, Yuto MIYAHARA², Kohei MIYAZAKI^{1,2,3}, Takeshi ABE^{1,2,3}

¹Graduate school of Global Environmental Studies, Kyoto University, ²Graduate school of Engineering, Kyoto University, ³Element Strategy Initiative for Catalysts & Batteries, Kyoto University

F1-13-P34

Conversion-Type Reaction Mechanism of MF₃ (M = Fe, Ti) Cathode for Li-Ion Battery: First-Principles Calculations

Tatsuya TAKAHASHI¹, Hiroyoshi MOMIDA^{1,2}, Tamio OGUCHI^{1,2}

¹The Institute of Scientific and Industrial Research, Osaka University, ²Elements Strategy Initiative for Catalysts and Batteries, Kyoto University

F1-13-P35

Comparative study of electrochemical behavior of micro-Sn and nano-Sn negative electrodes for Na-ion batteries

Mika FUKUNISHI^{1,2}, Tatsuo HORIBA^{1,2}, Kei KUBOTA^{1,2}, Shinichi KOMABA^{1,2}

¹Tokyo University of Science, ²ESICB, Kyoto University

F1-13-P36

Polyanionic Compounds as Positive Electrode Materials for K-Ion Batteries

Tomooki HOSAKA¹, Tomoaki SHIMAMURA¹, Kei KUBOTA^{1,2}, Shinichi KOMABA^{1,2}

¹Tokyo University of Science, ²ESICB, Kyoto University

F1-13-P37

Impact of metal-substitution in O3-type NaNi_{1/2}Mn_{1/2}O₂ for Na-Ion Battery

Naoya FUJITANI¹, Yusuke YODA¹, Kazutoshi KUROKI¹, Kei KUBOTA^{1,2}, Shinichi KOMABA^{1,2}

¹Tokyo University of Science, ²ESICB, Kyoto University

F1-13-P38

Ca substitution effect on layered P3 and P2-type Na_xCoO₂

Yuji ISHADO¹, Hirona HASEGAWA², Shigeto OKADA^{3,4}, Minoru MIZUHATA², Hideshi MAKI², Masaki MATSUI^{2,4}

¹Interdisciplinary Graduate School of Engineering Sciences, Kyushu University, ²Department of Chemical Science and Engineering, Kobe University, ³Institute for Materials Chemistry and Engineering, Kyushu University, ⁴Elements Strategy Initiative for Catalyst and Batteries (ESICB), Kyoto University

F1-13-P39

First-Principles Study on Cation-Disordered Rock-Salt Type Cathode $\text{Li}_{2.4}\text{M1}_{0.8}\text{M2}_{0.8}\text{O}_4$ (M1, M2 = Ti, Cr, and Mn) for Li-Ion Batteries

Motoyuki HAMAGUCHI¹, Hiroyoshi MOMIDA^{1,2}, Tamio OGUCHI^{1,2}

¹Institute of Scientific and Industrial Research, Osaka University, ²Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University

F1-13-P40

Effects of Magnesium-Organo-Haloaluminate Complex in Magnesium Ion Battery Electrolytes: A Car-Parrinello Molecular Dynamics Study

Ashu CHOUDHARY, Keitaro SODEYAMA, Yoshitaka TATEYAMA
NIMS

F1-13-P41

Lithium Diffusion Mechanism in Highly Concentrated Electrolytes via First-Principles Molecular Dynamics Sampling

Yang SUN¹, Keitaro SODEYAMA^{2,3}, Yuki YAMADA^{3,4}, Atsuo YAMADA^{3,4}, Yoshitaka TATEYAMA^{1,2}

¹Center for Green Research on Energy and Environmental Materials (GREEN) & International Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), ²Center for Materials Research Information Integration (cMI2), Research and Services Division of Materials Data and Integrated System (MaDIS), NIMS, ³Elements Strategy Initiative for Catalysts & Batteries (ESICB), Kyoto University, ⁴Department of Chemical System Engineering, The University of Tokyo

F1-13-P42

Na^+ Conducting Na_3SbS_4 -Based Solid Electrolytes

Akitoshi HAYASHI, Fumika TSUJI, Naoki MASUZAWA, So YUBUCHI, Chie HOTEHAMA, Atsushi SAKUDA, Masahiro TATSUMISAGO
Osaka Prefecture University

F1-13-P43

Improving intrinsic and surface of traditional graphene oxide as active material for supercapacitors electrodes

Sarawudh NATHABUMROONG¹, Saroj RUJIRAWAT¹, Rattikorn YIMNIRUN³, Adisorn TUANTRANONT²

¹Suranaree University of Technology, ²National Electronics and Computer Technology Center, ³Vidyasirimedhi Institute of Science and Technology

F1-13-P44

Phenolic Resin Derived Hard Carbon as Negative Electrode for High-Energy Sodium- and Potassium-Ion Batteries

Azusa KAMIYAMA¹, Kei KUBOTA¹, Shun FUJIMURA¹, Soshi SHIRAIISHI², Hidehiko TSUKADA³, Shinishi KOMABA¹

¹Tokyo University of Science, ²Gunma University, ³AION Co., Ltd.

F1-13-P45

Synthesis of molybdenum disulfide/ nitrogen-doped reduced graphene oxide nanocomposite for high performance supercapacitors

Wipakorn RITTISUT
Suranaree University of Technology

F1-13-P46

$\text{K}_2[(\text{VO})_2(\text{HPO}_4)_2(\text{C}_2\text{O}_4)]$ as 4 V Electrode Material for K-Ion Batteries

Shahul Hameed ABDULRAHMAN¹, Akihiro KATOI¹, Kei KUBOTA^{1,2}, Shinichi KOMABA^{1,2}

¹Tokyo University of Science, ²ESICB, Kyoto University

F1-13-P47

Multiple Adsorption Modes and Decomposition Pathways of Carbonate Electrolyte Molecules at $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ Cathode Interfaces: Ab Initio Study

Yoshitaka TATEYAMA¹, Keisuke USHIROGATA³, Ganes SHUKRI^{1,2}, Yukihiro OKUNO³

¹National Institute for Materials Science, ²Kyoto University, ³FUJIFILM Corporation

December 11, 2019

Symposium F-2Catalysis and Catalyst Materials for Energy
and Environment

[Organizers]

Tetsuya SHISHIDO (Tokyo Metropolitan University)
Wen-Yueh YU (National Taiwan University)
Kevin C.-W. WU (National Taiwan University)
Ning YAN (National University of Singapore)
Katsutoshi NAGAOKA (Nagoya University)
Yutaka AMAO (Osaka City University)
Koji OHTA (Kyoto University)

December 11, 2019

Oral Session 1

Time 9:00–12:15 Room Work-5

Chairperson Tetsuya SHISHIDO

Opening Talk
Tetsuya Shishido
9:00–9:05

F2-11-K01 ▶ Keynote 9:05–9:45

Single-atom catalysts for energy and environmental
applications

Ning YAN

National University of Singapore

F2-11-002 9:45–10:00

Charge transfer process of WO_x-modified Ti-HAp under
UV illuminationKana ISHISONE¹, Toshihiro ISOBE¹, Sachiko MATSUSHITA¹,
Masato WAKAMURA², Mitsutake OSHIKIRI³,
Akira NAKAJIMA¹¹Tokyo Institute of Technology, ²Fujitsu Laboratories Ltd.,³National Institute of Materials Science

F2-11-003 10:00–10:15

Vibration-driven reaction of CO₂ on Cu surfacesTakumi IMABAYASHI¹, Jiamei QUAN², Taijun KOZARASHI¹,
Tomoyasu MOGI¹, Takahiro KONDO^{2,3}, Junji NAKAMURA^{2,3}¹Graduate School of Pure and Applied Sciences, Universityof Tsukuba, ²Faculty of Pure and Applied Sciences,University of Tsukuba, ³Tsukuba Research Center for
Energy Materials Science (TREMS), University of Tsukuba

F2-11-004 10:15–10:30

Electronic Factors Affecting Surface Oxygen Vacancy
Formation Energies on Metal OxidesKenichi SHIMIZU^{1,2}, Takashi TOYAO^{1,2}, Takashi KAMACHI^{2,3},
Yoyo HINUMA⁴¹Institute for Catalysis, Hokkaido University, ²ESICB, Kyoto
University, ³Department of Life, Environment and Materials
Science, Fukuoka Institute of Technology, ⁴Center for
Frontier Science, Chiba University

Break
10:30–10:45

F2-11-I05 ▶ Invited 10:45–11:15

Metal-Organic Frameworks (MOFs)-Derived Nanomaterials
for Catalytic Conversion of Lignocellulosic Biomass

Kevin C.-W. WU

National Taiwan University

F2-11-006 11:15–11:30

Purification of automotive exhaust gas over Pd catalyst
supported on Ca₂AlMnO₅₊₆Saburo HOSOKAWA^{1,2}, Yudai OSHINO², Hiroyuki ASAKURA^{1,2},
Kentaro TERAMURA^{1,2}, Tsunehiro TANAKA^{1,2}¹Element Strategy Initiative for Catalysts & Batteries
(ESICB), Kyoto University, ²Department of Molecular
Engineering, Graduate School of Engineering, Kyoto
University

F2-11-007 11:30–11:45

Synergistic Effect between Isolated Electron-Rich Pt and
Co for Automotive Exhaust PurificationKatsutoshi SATO^{1,3}, Ayano ITO², Hiroyuki TOMONAGA²,
Homare KANEMATSU², Yuichiro WADA², Hiroyuki ASAKURA¹,
Saburo HOSOKAWA¹, Tsunehiro TANAKA¹,
Katsutoshi NAGAOKA^{1,3}¹Kyoto University, ²Oita University, ³Nagoya University

F2-11-008 11:45–12:00

Effect of Zeolite Topology on Cu Species in Cu-Zeolite
Catalysts for NO Direct DecompositionYusuke OHATA¹, Takahiko MOTOKI^{1,2}, Masaru OGURA^{1,2}¹Institute of Industrial Science, the University of Tokyo, ²Unit
of Elements Strategy Initiative for Catalysts & Batteries,
Kyoto University

F2-11-009 12:00–12:15

A possible mechanism for high turnover frequency CO-
NO reactions over nanometric Rh overlayer catalystsHirosi YOSHIDA^{1,2}, Yusuke KUZUHARA¹, Kenichi KOIZUMI^{2,3},
Masahiro EHARA^{2,4}, Mauro BOERO⁵, Akinori MATSUMOTO¹,
Satoshi MISUMI¹, Junya OHYAMA^{1,2}, Masato MACHIDA^{1,2}¹Kumamoto University, ²Kyoto University, ³Riken, ⁴Institute
for Molecular Science, ⁵University of Strasbourg

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 11, 2019

Oral Session 2
Time 14:00–16:10 **Room** Work-5

Chairperson Kevin C.-W. WU

F2-11-K10 ▶ Keynote 14:00–14:40

Ammonia synthesis under Mild Conditions

Ping CHEN

Dalian Institute of Chemical Physics

F2-11-I11 ▶ Invited 14:40–15:10

Heterogeneous Catalysis of Porous Ionic Crystals Based on Polyoxometalates

Sayaka UCHIDA

The University of Tokyo

F2-11-012 15:10–15:25

Acid-durable Electride with Layered Ruthenium for Ammonia Synthesis: Boosting the Activity via Selective Etching

Jiang LI¹, Jiazhen WU¹, Haiyun WANG², Yangfan LU¹, Tiannan YE¹, Masato SASASE¹, Xiaojun WU², Masaaki KITANO¹, Takeshi INOSHITA¹, Hideo HOSONO¹
¹Research Center for Element Strategy, Tokyo Institute of Technology, ²Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China

F2-11-013 15:25–15:40

Electride Materials for Advanced Catalytic Application

Tian-Nan YE

Tokyo Institute of Technology

F2-11-014 15:40–15:55

Carbon Dioxide Hydrogenation to Formic Acid Driven by Nano-structured Metal Catalysts

Kohsuke MORI^{1,2,3}, Taiki SANO¹, Shinya MASUDA¹, Hiromi YAMASHITA^{1,3}
¹Osaka University, ²JST-PRESTO, ³ESICB, Kyoto University

F2-11-015 15:55–16:10

Pt-Fe surface alloy active for CO room-temperature oxidation

Teng MA¹, Yaqin WANG^{1,2}
¹Shenyang Agricultural University, ²Shenyang Ligong University

December 11, 2019

Oral Session 3
Time 16:30–18:40 **Room** Work-5

Chairperson Katsutoshi NAGAOKA

F2-11-K16 ▶ Keynote 16:30–17:10

Transition Metal-Catalyzed Reduction of Molecular Dinitrogen into Ammonia under Ambient Conditions

Yoshiaki NISHIBAYASHI

The University of Tokyo

F2-11-I17 ▶ Invited 17:10–17:40

Design of Heteropolytungstates for Water Oxidation Catalysis

Masahiro SADAKANE

Hiroshima University

F2-11-018 17:40–17:55

Improvement of Hydrogen Oxidation Reaction in Alkaline Solutions by Modification of Pt/C Catalyst

Junya OHYAMA¹, Keiichi OKUBO³, Atsushi SATSUMA^{2,3}
¹Kumamoto University, ²Kyoto University ESICB, ³Nagoya University

F2-11-019 17:55–18:10

The OER/ORR Mechanism Including Redox Cycle of Perovskite Oxides for Secondary Metal-Air Batteries

Oyunbileg GALINDEV^{1,2}, Tatsuya TAKEGUCHI^{1,3}, Koichi UI¹, Enkhsaruul BYAMBAJAV²
¹Iwate University, ²National University of Mongolia, ³ESICB

F2-11-020 18:10–18:25

 Interaction of O₂, CO₂, and H₂O with Perovskite Surfaces. Insights from the Theory.

Aleksandar STAYKOV¹, Tatsumi ISHIHARA¹, John KILNER²
¹Kyushu University, ²Imperial College London

F2-11-021 18:25–18:40

Mechanistic Investigation in Reverse Water-Gas Shift Reaction over Platinum Catalysts Supported on Various Metal Oxides

Akira YAMAMOTO¹, Yuqiang DAI¹, Taiki WATANABE¹, Hisao YOSHIDA^{1,2}
¹Graduate School of Human and Environmental Studies, Kyoto University, ²Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University

December 11, 2019

Poster Session

Time 12:15–14:00 Room Trade-0

F2-11-P01**Catalytic Combustion of Diesel Soot over Fe and Ag-doped Manganese Oxide Catalyst**Yasutaka KUWAHARA^{1,2}, Akihiro FUJIBAYASHI¹, Genki KATO¹, Kohsuke MORI^{1,2,3}, Hiromi YAMASHITA^{1,2}¹Osaka University, ²Unit of Elements Strategy Initiative for Catalysts & Batteries (ESICB), ³JST, PRESTO**F2-11-P02****Shape Controlled CoO_x/CeO₂ Catalyst in Diesel Soot Combustion**Kohsuke MORI¹, Hiroataka JIDA¹, Yasutaka KUWAHARA^{1,2}, Hiromi YAMASHITA^{1,2}¹Osaka University, ²ESICB Kyoto University, ³JST-PRESTO**F2-11-P03****Ultrathin Oxide Films as Potential Catalysts for NO-CO Elimination: A DFT Study**Hiroaki KOGA¹, Kohei TADA², Akihide HAYASHI³, Yoshinori ATO³, Mitsutaka OKUMURA^{1,3}¹ESICB, Kyoto University, ²Research Institute of Electrochemical Energy, AIST, ³Department of Chemistry, Osaka University**F2-11-P04****Pd/CoAl₂O₄/Al₂O₃ Prepared by Galvanic Deposition – Promotion of Reduction-Oxidation Steps of Pd Particle during Methane Combustion**Atsushi SATSUMA^{1,2}, Yuji MAHARA¹, Takumi TOJO¹, Kazumasa MURATA¹, Junya OHYAMA^{1,2,3}¹Nagoya University, ²ESICB Kyoto University, ³Kumamoto University**F2-11-P05****Methanolysis of ammonia borane over supported Pd-Au alloy catalysts**Tetsuya SHISHIDO^{1,2,3,4}, Mitsuhiro TOMINAGA¹, Hiroshi MIURA^{1,2,4}¹Department of Applied Chemistry for Environment, Graduate School of Engineering, Tokyo Metropolitan University, ²Research Center for Hydrogen Energy-based Society, Tokyo Metropolitan University, ³Research Center for Gold Chemistry, Tokyo Metropolitan University, ⁴Elements Strategy Initiative for Catalysts & Batteries, Kyoto University**F2-11-P06****Preparation of ZrO₂/C cathode catalysts as an alternative of Pt/C for polymer electrolyte fuel cells**Jun KUBOTA^{1,2}, Masako MATSUYAMA¹¹Fukuoka University, ²ESICB, Kyoto University**F2-11-P07****Automated Structural and Reaction Pathway Searches Toward Theoretical Cluster Catalysis**Takeshi IWASA^{1,2,3}, Takaaki SATO⁴, Makito TAKAGI⁴, Min GAO⁵, Yusuke KONDO³, Rina TAKAHARA⁴, Hirono MOHRI⁴, Andrey LYALIN², Masato KOBAYASHI^{1,2,3,6}, Ken-ichi SHIMIZU^{3,5}, Satoshi MAEDA^{1,2,3}, Tetsuya TAKETSUGU^{1,2,3,4}¹Department of Chemistry, Faculty of Science, Hokkaido University, ²WPI-ICReDD, Hokkaido University, ³ESICB, Kyoto University, ⁴Graduate School of Chemical Sciences and Engineering, Hokkaido University, ⁵Institute for Catalysis, Hokkaido University, ⁶JST-PRESTO**F2-11-P08****Adsorption and Activation of Methane on the (110) Surface of IrO₂**Yuta TSUJI, Kazunari YOSHIKAWA
Kyushu University**F2-11-P09****Construction of Surface Model Calculation Database and Its Usage for Catalytic Activity Prediction: A Case Study for Methane Steam Reforming**Masato KOBAYASHI^{1,2,3}, Haruka ONODA⁴, Tetsuya TAKETSUGU^{1,2,3}¹Faculty of Science, Hokkaido University, ²WPI-ICReDD, Hokkaido University, ³ESICB, Kyoto University, ⁴Graduate School of Chemical Sciences and Engineering, Hokkaido University**F2-11-P10****Preparation of Ru/Complex-rare-earth Oxide for Efficient Ammonia Synthesis**Yuta OGURA¹, Shin-ichiro MIYAHARA¹, Takahiro ASAI², Katsutoshi SATO³, Katsutoshi NAGAOKA¹¹Nagoya University, ²Oita University, ³Kyoto University**F2-11-P11****Effect of Oxygen Non-Stoichiometry of LaNiO₃₋₆ on Oxygen Reduction and Evolution Reaction Activities**Hiroyuki TANAKA¹, Hiroyuki ASAKURA^{1,2}, Saburo HOSOKAWA^{1,2}, Kentaro TERAMURA^{1,2}, Tsunehiro TANAKA^{1,2}¹Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, ²Elements Strategy Initiative for Catalysts & Batteries (ESICB), Kyoto University**F2-11-P12****Three-way catalytic reaction using FeNbO₄ as catalyst support**Kenya ONISHI¹, Saburo HOSOKAWA^{1,2}, Hiroyuki ASAKURA^{1,2}, Kentaro TERAMURA^{1,2}, Tsunehiro TANAKA^{1,2}¹Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, ²Element Strategy Initiative for Catalysts & Batteries (ESICB), Kyoto University

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

F2-11-P13
Particle size effect on CO oxidation over Pd/Al₂O₃ with different alumina crystalline phase

Kazumasa MURATA¹, Eleen ELEEDA¹, Junya OHYAMA^{2,3}, Yuta YAMAMOTO⁴, Shigeo ARAI⁴, Atsushi SATSUMA^{1,3}

¹Graduate School of Engineering, Nagoya University, ²Faculty of Advanced Science and Technology, Kumamoto University, ³Unit of Elements Strategy Initiative for Catalysts & Batteries, Kyoto University, ⁴Institute of Materials and Systems for Sustainability, Nagoya University

F2-11-P14
Development of Pd Catalyst Supported on Sr-Ti Mixed Oxide for Purifying Automotive Exhaust Gases

Chikara WATANABE¹, Saburo HOSOKAWA^{1,2}, Hiroyuki ASAKURA^{1,2}, Kentaro TERAMURA^{1,2}, Tsunehiro TANAKA^{1,2}

¹Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, ²Element Strategy Initiative for Catalysts & Batteries (ESICB), Kyoto University

F2-11-P15
Activity of Silica-Coated Pt Cathode Catalysts with Low Ionomer Loading for PEFCs under Low Humidity Conditions

Masaki GOTO, Sakae TAKENAKA
Doshisha University

F2-11-P16
Improvement of the Durability of Pt Cathode Catalysts for PEFCs using Titanium Oxide Nanosheets

Sakae TAKENAKA^{1,2}, Tomohiro SUZUKI¹

¹Doshisha University, ²Kyoto University

F2-11-P17
DFT Calculations Analysis of Catalytic Activity Modifications with Electric Field

Katsuhiko WAKAMATSU, Tepei OGURA
Kwansei Gakuin University

F2-11-P18
Origin of (NO)₃ Formation on Cu(111) from Density Functional Theory Calculations.

Yoshitada MORIKAWA^{1,3}, Thanh Ngoc PHAM^{1,2}, Kouji INAGAKI^{1,3}, Do Ngoc SON², Ikutaro HAMADA^{1,3}, Yuji HAMAMOTO^{1,3}

¹Osaka University, ²Ho Chi Minh City University of Technology, VNU-HCM, ³ESICB, Kyoto University

F2-11-P19
Why Does Not Only the Rh₁₃⁺ Cluster Reduce Nitrogen Oxides?

Naoki HARUTA^{1,2,3}, Sho FUKUSHIMA^{1,2}, Wataru OTA^{1,2}, Tohru SATO^{1,2,3}

¹Fukui Institute for Fundamental Chemistry, Kyoto University, Japan, ²Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Japan, ³Unit of Elements Strategy Initiative for Catalysts & Batteries, Kyoto University, Japan

F2-11-P20
Density-Functional Tight-Binding Study on Oxygen Vacancy Diffusion in Ceria Systems

Aditya Wibawa SAKTI^{1,2}, Chien-Pin CHOU², Hiromi NAKAI^{1,2,3}

¹Element Strategy Initiative for Catalysts and Batteries, Kyoto University, Kyoto, 615-8520, Japan, ²WISE Waseda University, Tokyo, 169-8555, Japan, ³Department of Chemistry and Biochemistry, Waseda University, Tokyo, 169-8555, Japan

F2-11-P21
Gold and Gold-Palladium Nanoflower Catalysts with High Catalytic Activity for Alcohol Oxidation

Yoshiro IMURA¹, Ryota AKIYAMA¹, Masami TANAKA¹, Haruna SAITO¹, Clara MORITA-IMURA², Takeshi KAWAI¹

¹Tokyo University of Science, ²Ochanomizu University

F2-11-P22
Local structure and three-way catalysis of thermally aged Cu/Al₂O₃

Taiki HIRAKAWA¹, Hiroshi YOSHIDA^{2,3}, Yushi SHIMOKAWA¹, Wakana TOKUZUMI¹, Junya OHYAMA^{2,3}, Masato MACHIDA^{2,3}

¹Department of Applied Chemistry and Biochemistry, Graduate School of Science and Technology, Kumamoto University, ²Division of Materials Science and Chemistry, Faculty of Advanced Science and Technology, Kumamoto University, ³Unit of Elements Strategy Initiative for Catalysts & Batteries, Kyoto University

F2-11-P23
***In situ* Reflectance Spectroscopy for the Real-Time Observation of Redox Dynamics of Pd Supported on CeO₂-ZrO₂**

Ayumi FUJIWARA¹, Yuki UCHIDA¹, Riichiro KAKEI¹, Hiroshi YOSHIDA^{2,3}, Junya OHYAMA^{2,3}, Masato MACHIDA^{2,3}

¹Graduate School of Science and Technology, Kumamoto University, ²Division of Materials Science and Chemistry, Faculty of Advanced Science and Technology, ³Unit of Elements Strategy Initiative for Catalysts & Batteries, Kyoto University

F2-11-P24
Enhanced Photocatalytic Activity of Perovskite NaNbO₃ by Oxygen Vacancies Engineering

Bian YANG, Jihong BIAN, Lei WANG, Jianwei WANG, Yaping DU, Zhiguang WANG, Chao WU, Yaodong YANG
Xi'an Jiaotong University

F2-11-P25
Redox behavior and three-way catalytic activity of Rh-Fe/Al₂O₃

Kyoko FUJITA¹, Hiroyuki ASAKURA^{1,2}, Saburo HOSOKAWA^{1,2}, Kentaro TERAMURA^{1,2}, Tsunehiro TANAKA^{1,2}

¹Kyoto University, ²ESICB, Kyoto University

F2-11-P26

Effect of Zn species in Ag-loaded Zn-modified ZnTa₂O₆ for Photocatalytic conversion of CO₂ by H₂O

Shuying WANG¹, Kentaro TERAMURA^{1,2}, Saburo HOSOKAWA^{1,2}, Hiroyuki ASAKURA^{1,2}, Tsunehiro TANAKA^{1,2}

¹Kyoto University, ²Element Strategy Initiative for Catalysts & Batteries (ESICB), Kyoto University

F2-11-P27

Electron-rich Gold Clusters Stabilized by Polyvinylpyridines as Robust and Active Oxidation Catalysts

Atsushi MATSUO¹, Shingo HASEGAWA¹, Shinjiro TAKANO¹, Tatsuya TSUKUDA^{1,2}

¹Department of Chemistry, The University of Tokyo, ²Elements Strategy Initiative for Catalysis and Batteries (ESICB), Kyoto University

F2-11-P28

Theoretical Study on the Electronic Origin and Reaction Mechanism of Catalytic Nitric Oxide Reduction with Metal Clusters

Ryoichi FUKUDA¹, Kaho NAKATANI¹, Nozomi TAKAGI¹, Masahiro EHARA², Shigeyoshi SAKAKI¹

¹Kyoto University, ²Institute for Molecular Science

F2-11-P29

Ammonia Synthesis Mechanism using Ru-loaded Hydride Catalyst from First principles

Takuya NAKAO, Tomofumi TADA, Hideo HOSONO
Materials Research Center for Element Strategy, Tokyo Institute of Technology

F2-11-P30

Improving Catalytic Performance and Stability of Polymer-Stabilized Gold Clusters

Tatsuya TSUKUDA^{1,2}, Shingo HASEGAWA¹, Atsushi MATSUO¹, Koto HIRANO¹, Shinjiro TAKANO¹

¹The University of Tokyo, ²Kyoto University

F2-11-P31

Synthesis of metal-metal oxide hybrid clusters and their catalytic properties

Jun HIRAYAMA^{1,2}, Taku KOJIMA², Tomoki MATSUYAMA², Kanako SHIBATA², Mio TSUKADA², Hiroki MIURA^{1,3}, Tetsuya SHISHIDO^{1,3}, Hikaru TAKAYA⁴, Seiji YAMAZOE^{1,2,5}

¹Elements Strategy Initiative for Catalysts and Batteries, Kyoto University, ²Department of Chemistry, Graduate School of Science, Tokyo Metropolitan University, ³Department of Applied Chemistry, Graduate School of Urban Environmental Sciences, Tokyo Metropolitan University, ⁴Institute for Chemical Research, Kyoto University, ⁵Core Research for Evolutional Science and Technology, Japan Science and Technology Agency

F2-11-P32

Reaction Behavior of NO Molecule on 4d Metal Clusters M₁₃ and M₅₅ (M = Ru, Rh, Pd, and Ag); Theoretical Study

Nozomi TAKAGI¹, Ryoichi FUKUDA¹, Masahiro EHARA^{1,2}, Shigeyoshi SAKAKI^{1,3}

¹Elements Strategy Initiative for Catalysts and Batteries, Kyoto University, ²Institute for Molecular Science, ³Fukui Institute for Fundamental Chemistry, Kyoto University

F2-11-P33

Design of Intermetallic Electrides for Catalytic Ammonia Synthesis

Jiazhen WU¹, Jiang LI¹, Masaaki KITANO¹, Takeshi INOSHITA^{1,2}, Hideo HOSONO^{1,3}

¹Materials Research Center for Element Strategy, Tokyo Institute of Technology, ²National Institute for Materials Science, ³Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology

F2-11-P34

Plasmonic Molybdenum Oxide Microspheres for Complete Nitrogen Photofixation

Haoyuan BAI, Jianhua YANG, Jianfang WANG
The Chinese University of Hong Kong

F2-11-P35

Propene Oxidation by M₅₅ Cluster (M= Pd or Rh): Theoretical Study of Reaction Mechanism and Difference(s) between Pd and Rh

Bo ZHU, Masahiro EHARA, Shigeyoshi SAKAKI
Kyoto University

F2-11-P36

Effect of size and morphology of Ag nanoparticles modified on NaTaO₃ for photoreduction of CO₂ by H₂O

Xu XUANWEN¹, Kentaro TERAMURA^{1,2}, Hiroyuki ASAKURA^{1,2}, Saburo HOSOKAWA^{1,2}, Tsunehiro TANAKA^{1,2}

¹Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, ²ESICB, Kyoto University

F2-11-P37

CO Oxidation and NO Reduction on Pd-loaded Sr₃Fe₂O₇₋₆ Catalyst: A Theoretical Approach

Kuduva R. VIGNESH^{1,2}, Archana VELLOTH^{1,2}, Ryoichi FUKUDA^{2,3}, Saburo HOSOKAWA^{2,3}, Tsunehiro TANAKA^{2,3}, Masahiro EHARA^{1,2}

¹Institute for Molecular Science, ²ESICB, Kyoto University, ³Department of Molecular Engineering, Kyoto University

F2-11-P38

Theoretical Investigation on Structures and Bond Activation on Isolated and Supported Pt-Co Bimetallic Nanoclusters

Masahiro EHARA^{1,2}, Archana VELLOTH^{1,2}, Tao YANG^{1,2}, Ryoichi FUKUDA^{2,3}

¹Institute for Molecular Science, ²ESICB, Kyoto University, ³Department of Molecular Engineering, Kyoto University

Symposium A
 Symposium B
 Symposium C
 Symposium D
 Symposium E
 Symposium F
 Symposium G
 Symposium H
 Symposium I
 F2-11-P39

Ammonia decomposition reaction on the Ni supported various metal imides

 Kiya OGASAWARA¹, Kazuhisa KISHIDA¹, Masaaki KITANO^{1,2}, Hideo HOSONO¹
¹Materials and Structures Laboratory, Tokyo Institute of Technology, ²Precursory Research for Embryonic Science and Technology (PRESTO), Japan Science and Technology Agency (JST)

F2-11-P40

Importance of Pd Site in Hydrosilylation of Internal Alkynes by Palladium-Gold Alloy Catalyst

 Pei ZHAO¹, Tumpa SADHUKHAN^{1,2}, Anchalee JUNKAEW³, Hiroki MIURA^{2,4,5}, Tetsuya SHISHIDO^{2,4,5}, Masahiro EHARA^{1,2}
¹Institute for Molecular Science, Research Center for Computational Science, ²Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, ³National Nanotechnology Center (NANOTEC), Thailand Science Park, ⁴Department of Applied Chemistry, Graduate School of Urban Environmental Sciences, Tokyo Metropolitan University, ⁵Research Center for Hydrogen Energy-Based Society, Tokyo Metropolitan University

F2-11-P41

Redox behavior of Ni–Cu bimetallic alloy catalysts for automobile exhaust purification

 Hiroyuki ASAKURA^{1,2}, Saburo HOSOKAWA^{1,2}, Kentaro TERAMURA^{1,2}, Nozomi TAKAGI², Shigeyoshi SAKAKI^{2,3}, Tsunehiro TANAKA^{1,2}
¹Kyoto University, ²ESICB, Kyoto University, ³Fukui Institute for Fundamental Chemistry, Kyoto University

F2-11-P42

The change of electronic structure at the interface between Pt nanoparticles and the carbon support by the ion irradiation

 Hiroyuki OKAZAKI¹, Akira IDESAKI¹, Hiroshi KOSHIKAWA¹, Daiju MATSUMURA², Syunya YAMAMOTO¹, Yusunari MAEKAWA¹, Tetsuya YAMAKI¹
¹National Institutes for Quantum and Radiological Science and Technology, ²Japan Atomic Energy Agency

F2-11-P43

Mechanistic Analysis of Oxygen Vacancy Formation and Ionic Transport in Sr₃Fe₂O_{7-δ}

 Tadashi OTA, Hidetoshi KIZAKI, Yoshitada MORIKAWA
 Department of Precision Science and Technology,
 Graduate School of Engineering, Osaka University

December 11–13, 2019

Symposium F-3**Advancements in Thermoelectric Materials and Applications**

[Organizers]

Takao MORI (National Institute for Materials Science)
 Michihiro OHTA (National Institute of Advanced Industrial Science and Technology)
 Lidong CHEN (Shanghai Institute of Ceramics, Chinese Academy of Sciences)
 Franck GASCOIN (CRISMAT)
 Yuri GRIN (Max Planck Institute for Chemical Physics of Solids)
 Yuzuru MIYAZAKI (Tohoku University)
 Michitaka OHTAKI (Kyushu University)
 Jong-Soo RHYEE (Kyung Hee University)
 Jeff SNYDER (Northwestern University)
 Tsunehiro TAKEUCHI (Toyota Technological Institute)
 Takahiro YAMAMOTO (Tokyo University of Science)

December 11, 2019

Oral Session 1

Time 9:00–12:05 Room Work-2

Chairpersons Takao MORI, Johannes DE BOOR, Yaniv GELBSTEIN

F3-11-K01 ▶ Keynote 9:00–9:25

The Effect of Microstructure in Understanding the Electronic Properties of Complex MaterialsG. Jeffrey SNYDER
Northwestern

F3-11-I02 ▶ Invited 9:25–9:45

Phonon dispersion and scattering in thermoelectricsYanzhong PEI
Tongji University

F3-11-I03 ▶ Invited 9:45–10:05

New concept to effectively increase ZT and development of high-performance Si-Ge based thermoelectric materialsTsunehiro TAKEUCHI
Toyota Technological Institute

F3-11-I04 ▶ Invited 10:05–10:25

Topological and Anderson transition in thermoelectricityJong-Soo RHYEE
Kyung Hee University

F3-11-I05 ▶ Invited 10:25–10:45

Effect of Phonon Drag on Seebeck Coefficient Based on Linear Response Theory: Application to FeSb₂Masao OGATA¹, Hiroyasu MATSUURA¹, Hideaki MAEBASHI¹, Hidetoshi FUKUYAMA²¹Department of Physics, University of Tokyo, ²Science University of Tokyo

F3-11-I06 ▶ Invited 10:45–11:05

Optical Properties of Thermoelectric MaterialsPeng JIANG
Dalian Institute of Chemical Physics, Chinese Academy of Sciences

F3-11-007 11:05–11:20

Enhanced thermoelectric properties of Si-Ge by tuning boron concentration and dispersion of Au nanoparticle in Si-Ge matrix synthesized by high-pressure and low-temperature sintering processOmprakash MUTHUSAMY
Toyota Technological Institute

F3-11-008 11:20–11:35

Charge density wave and thermoelectric properties in Te-deficient InTe_{1-x} compoundsSong Yi BACK¹, Young-Kwang KIM², Hyunyoung CHO¹, Jong-Soo RHYEE¹¹Kyung Hee University, ²Pohang University of Science and Technology (POSTECH)

F3-11-009 11:35–11:50

Locally Distorted Structures with Multiple Anions Realize Ultralow Lattice Thermal ConductivityNaoki SATO¹, Norihide KURODA², Yukari KATSURA³, Ikuzo KANAZAWA², Kaoru KIMURA³, Takao MORI¹¹WPI-MANA and CFSN, National Institute for Materials Science, ²Tokyo Gakugei University, ³The University of Tokyo

F3-11-010 11:50–12:05

(Micro)Structure – Thermoelectric Properties Relationships In Mesostructured MnSi_{1.74} and β-FeSi₂ Prepared By Magnesio-reductionSylvain LE TONQUESSE¹, Valérie DEMANGE¹, Carmelo PRESTIPINO¹, Vincent DORCET¹, Loïc JOANNY¹, Quansheng GUO², David BERTHEBAUD², Takao MORI³, Mathieu PASTUREL¹¹Univ. Rennes, ²CNRS - Saint-Gobain - NIMS, LINK, ³National Institute for Materials Science (NIMS)

December 11, 2019

Oral Session 2

Time 14:00–16:00 Room Work-2

Chairpersons G. Jeffrey SNYDER, Tsunehiro TAKEUCHI

F3-11-K11 ▶ Keynote 14:00–14:25

Challenges Facing the Thermoelectrics CommunityZhifeng REN
University of Houston

F3-11-I12 ▶ Invited 14:25–14:45

Towards Magnesium-Silicide Based Thermoelectric Generators: Material Optimization, Contact Development and PrototypesJohannes DE BOOR
German Aerospace Center (DLR)

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

F3-11-013 14:45–15:00

Silicides for industrial heat waste recovery

David BERTHEBAUD¹, Quansheng GUO^{1,2}, Yuichi MICHIE², Franck GASCOIN³, Sylvain LE TONQUESSE⁴, Mathieu PASTUREL⁴, Takao MORI²

¹CNRS-Saint Gobain-NIMS, UMI 3629, Laboratory for Innovative Key Materials and Structures (LINK), National Institute for Materials Science, Tsukuba 305-0044, Japan, ²WPI-MANA & CFSN, NIMS, 1-1 Namiki, Tsukuba 305-0044, Japan, ³Laboratoire CRISMAT UMR 6508 CNRS ENSICAEN, France, ⁴Univ Rennes, CNRS, ISCR-UMR6226, F-35000, Rennes France

F3-11-014 15:00–15:15

Refinement of the Calculated Power Generation Characteristics of a Unileg-type Mg₂Si Thermoelectric Module Using Thermal-electric Analysis

Yuki SHIOJIMA, Takeaki HARADA, Kenki TANI, Tatsuya YAMASHITA, Daishi SHIOJIRI, Tsutomu IIDA
Tokyo University of Science

F3-11-015 15:15–15:30

Conversion Efficiency Of Colusite (Cu₂₆Nb₂Ge₆S₃₂)-Based Thermoelectric Element With Au-Based Diffusion Barrier

Raju CHETTY¹, Yuta KIKUCHI¹, Yohan BOUYRIE¹, Priyanka JOOD¹, Atsushi YAMAMOTO¹, Koichiro SUEKUNI², Michihiro OHTA¹

¹National Institute of Advanced Industrial Science and Technology, ²Kyushu University

F3-11-016 15:30–15:45

Measurement of thermophysical property distribution by pulsed light heating thermoreflectance method with high spatial resolution

Tetsuya BABA, Naoki SATO, Takahiro BABA, Takao MORI
National Institute of Materials Science

F3-11-017 15:45–16:00

Perspectives of ultra-high temperature thermoelectric materials and applications

Takao MORI
National Institute for Materials Science (NIMS)

December 11, 2019
Oral Session 3
Time 16:30–18:30 **Room** Work-2

Chairpersons Zhifeng REN, Jong-Soo RHYEE

F3-11-118 ▶ Invited 16:30–16:50

Chalcogenides based thermoelectric materials for power generation

Yaniv GELBSTEIN
Ben-Gurion University

F3-11-119 ▶ Invited 16:50–17:10

Thermoelectric Modules for Near Room-temperature Uses Based on N-type Mg₃Sb_{1.5}Bi_{0.5} Materials and P-type Bi_{0.48}Sb_{1.52}Te₃

Huaizhou ZHAO
Institute of Physics, Chinese Academy of Sciences

F3-11-120 ▶ Invited 17:10–17:30

Investigation on the stability of liquid-like thermoelectric materials and modules

Pengfei QIU¹, Xun SHI¹, Lidong CHEN¹, Jeffrey SNYDER²
¹Shanghai Institute of Ceramics, Chinese Academy of Sciences, ²Department of Materials Science and Engineering, Northwestern University

F3-11-021 17:30–17:45

Development Of High-Efficiency Segmented Thermoelectric Systems For Space Applications

Kathleen LEE¹, Jean-Pierre FLEURIAL¹, Sabah BUX¹, Fivos DRYMIOTIS¹, Kurt STAR¹, Ike CHI¹, Kevin YU¹, Obed VILLALPANDO¹, Billy LI¹, Kevin SMITH¹, Dean CHEIKH¹, David UHL¹, Chen-Kuo HUANG¹, Michell ARANDA¹, David NEFF¹, Sutinee SUJITTOSAKUL¹, Emmanuelle DESPAGNET-AYOUB¹, Jong-Ah PAIK¹, Samad FIRDOSY¹, Knut OXNEVUT¹, Vilupanur RAVI^{1,2}, Frances HURWITZ³, Dongming ZHU³, Haiquan GUO³, Gustavo COSTA³, Kang LEE³, Jessica CASHMAN³, Zi Kui LIU⁴, Jorge PAZ SOLDAN PALMA⁴, Yi WANG⁴, XiaoYu CHONG⁴
¹NASA Jet Propulsion Laboratory, ²California State Polytechnic University Pomona, ³NASA Glenn Research Center, ⁴Pennsylvania State University

F3-11-022 17:45–18:00

Development of Thermal Diodes using Unusual Thermoelectric Properties of Ag₂Ch (Ch = S, Se, Te)

Keisuke HIRATA, Takuya MATSUNAGA, Masaharu MATSUNAMI, Tsunehiro TAKEUCHI
Toyota Technological Institute

F3-11-023 18:00–18:15

Examination of Fabrication Condition of Thermoelectric Conversion Devices Using Porous Thermoelectric Materials

Yasutaka HASHIMOTO¹, Makoto SASAKI¹, Yohei HIYAMA¹, Takatoshi NAGANO², Teruyuki IKEDA²
¹Graduate School of Science and Engineering, Ibaraki University, ²Department of Materials Science and Engineering, College of Engineering, Ibaraki University

F3-11-024 18:15–18:30

Development of a New Heat Flow Switching Device

Takuya MATSUNAGA, Keisuke HIRATA, Masaharu MATSUNAMI, Tsunehiro TAKEUCHI
Toyota Technological Institute

December 12, 2019

Oral Session 4**Time** 9:00–12:05 **Room** Trade-1Chairpersons Franck GASCOIN, Dario NARDUCCI,
Prashun GORAI**F3-12-K01** ▶ Keynote 9:00–9:25**Chemical bonding and thermoelectrics**Yuri GRIN
Max-Planck-Institut für Chemische Physik fester Stoffe**F3-12-I02** ▶ Invited 9:25–9:45**How Far Can Chemists Go Toward High ZT**Ling CHEN, Li-Ming WU
Beijing Normal University**F3-12-I03** ▶ Invited 9:45–10:05**Combined use of Alloying and Interstitials to Enhance the Performance of TiNiSn-based Half-Heuslers**Jan-Willem BOS¹, Sonia BARCZAK¹, Robert QUINN¹,
Srinivas POPURI¹, John HALPIN², Donald MACLAREN²,
Kamil DOMOSUD³, Keith REFSON³
¹Heriot-Watt University, ²University of Glasgow, ³Royal Holloway University London**F3-12-I04** ▶ Invited 10:05–10:25**From bulk to film: largely enhanced thermoelectric performance in full Heusler systems**Ernst BAUER¹, Bernhard HINTERLEITNER¹, Takao MORI²,
Xingqiu CHEN³
¹TU Wien, ²Institute for Materials Science, NIMS, ³Shenyang National Laboratory for Materials Science**F3-12-005** 10:25–10:40**Ru-substitution effects on the crystal and electronic structures, and thermoelectric properties of half-Heusler-type VFeSb compounds**Yi HUANG, Kei HAYASHI, Yuzuru MIYAZAKI
Tohoku University**F3-12-I06** ▶ Invited 10:40–11:00**CoGe_{1.5}Te_{1.5} Skutterudites for Thermoelectric Performance**Kuei-Hsien CHEN¹
¹Institute of Atomic and Molecular Sciences, Academia Sinica, ²Center for Condensed Matter Sciences, National Taiwan University, ³Taiwan International Graduate Program, Academia Sinica**F3-12-007** 11:00–11:15**Power factor and wettability of the filled skutterudite Sm_y(Fe_xNi_{1-x})₄Sb₁₂**Giovanna LATRONICO
Shibaura Institute of Technology**F3-12-008** 11:15–11:30**Effect of non-equilibrium processing on the synthesis and thermoelectric properties of skutterudites and half Heusler compounds**Alberto CASTELLERO¹, Francesco AVERSANO¹,
Stefano BOLDRINI², Alberto FERRARIO², Carlo FANCIULLI³,
Marcello BARICCO¹
¹University of Turin, ²CNR – ICMATE, Padova, ³CNR – ICMATE, Lecco**F3-12-I09** ▶ Invited 11:30–11:50**Exceptional Thermoelectric Performance of Polycrystalline SnSe Materials**In CHUNG^{1,2}
¹Seoul National University, ²Nanoparticle Research Center, Institute for Basic Science**F3-12-010** 11:50–12:05**Study on thermoelectric properties of co-evaporated Sn-Se films with different phase formations**Guojian LI, Baohai JIA, Shiyang LIU, Shan LIU,
Yaoyao ZHOU, Qiang WANG
Northeastern University

December 12, 2019

Oral Session 5**Time** 14:00–16:10 **Room** Work-2

Chairpersons Yuri GRIN, In CHUNG

F3-12-I11 ▶ Invited 14:00–14:20**Ionic Pnictides for High Temperature Applications**Franck GASCOIN
CRISMAT laboratory, CNRS, ENSICAEN**F3-12-I12** ▶ Invited 14:20–14:40**Beyond the Known: Computational Discovery of New n-type Zintl Thermoelectric Materials**Prashun GORAI
Colorado School of Mines**F3-12-I13** ▶ Invited 14:40–15:00**Thermoelectric Properties of Ternary Thallium Tellurides**Holger KLEINKE
University of Waterloo**F3-12-I14** ▶ Invited 15:00–15:20**Silicon Reloaded: Novel Perspectives of Si as a Thermoelectric Material**Dario NARDUCCI
University of Milano Bicocca

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

F3-12-115 ▶ Invited 15:20–15:40

Ag₂Se and PbTe thermoelectrics- High performance materials and modules for room temperature to mid-temperature applications.
Priyanka JOOD¹, Atsushi YAMAMOTO¹, G. Jeffrey SNYDER², Mercuri G. KANATZIDIS^{3,4}, Michihiro OHTA¹
¹Research Institute for Energy Conservation, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, 305-8568, Japan, ²Department of Materials Science & Engineering, Northwestern University, Evanston, 60208, USA, ³Department of Chemistry, Northwestern University, Evanston, 60208, USA, ⁴Materials Science Division, Argonne National Laboratory, Argonne, 60439, USA

F3-12-016 15:40–15:55

Enhancing the transport properties of Bi₂Te_{3-x}Se_x alloys for thermoelectric power generation applications via melt-spinning
Omer MEROZ
Ben Gurion University of the Negev

F3-12-017 15:55–16:10

Enhanced thermoelectric performance of p-type Bi₂Te₃-based alloys reprocessed from commercial ingot by nano SiC dispersion
Bowen CAI
Tsinghua University

December 13, 2019

Oral Session 7

Time 9:00–12:05 **Room** Work-2

Chairpersons Koji MIYAZAKI, Kedar HIPPALGAONKAR, Naohito TSUJII

F3-13-K01 ▶ Keynote 9:00–9:25

Synergistic control of electrical and thermal transport property in thermoelectric nanocomposites
Jing-Feng LI
Tsinghua University

F3-13-I02 ▶ Invited 9:25–9:45

Link the relationship between structure and thermoelectric property through atomic observation
Zhigang CHEN
University of Southern Queensland

F3-13-I03 ▶ Invited 9:45–10:05

A high-throughput approach to thermoelectric materials with enhanced properties in complex material systems
Teruyuki IKEDA
Ibaraki University

F3-13-I04 ▶ Invited 10:05–10:25

Defects And Their Influence On The Thermoelectric Properties Of Materials: An *Ab Initio* Study
Philippe JUND, Alexandre BERCHE
University of Montpellier

F3-13-I05 ▶ Invited 10:25–10:45

First-Principles Thermoelectric Calculations of Magnetic Semiconductors
Hirokazu TAKAKI^{1,2}, Kazuaki KOBAYASHI², Masato SHIMONO², Nobuhiko KOBAYASHI¹, Kenji HIROSE³, Naohito TSUJII², Takao MORI²
¹University of Tsukuba, ²National Institute for Materials Science, ³NEC corporation

F3-13-I06 ▶ Invited 10:45–11:05

First Principles Simulations of Thermoelectric Transport in n-type PbTe
Ivana SAVIC¹, Jiang CAO^{1,2}, Jose D. QUERALES-FLORES¹, Stephen FAHY^{1,3}
¹Tyndall National Institute, Cork, T12 R5CP, Ireland, ²Department of Electronic and Optical Engineering, Nanjing University of Science and Technology, Nanjing, 210094, China, ³Department of Physics, University College Cork, Cork, T12 K8AF, Ireland

F3-13-007 11:05–11:20

Development of high-performance thermoelectric materials of rock-salt IV-VI compounds guided by large-scale experimental data and first-principle calculation
Takushi KODANI¹
¹The University of Tokyo, ²National Institute for Materials Science (NIMS)

F3-13-008 11:20–11:35

First-Principles Study of Thermoelectric Properties of Iodide Perovskite
Satoshi IIKUBO, Kumiko YAMAMOTO, Shoya KAWANO, Masayuki MORIMOTO, Koji MIYAZAKI
Kyushu Institute of Technology

F3-13-009 11:35–11:50

Discovery of Colossal Seebeck Effect in Metallic Cu₂Se
Dogyun BYEON¹, Robert SOBOTA¹, Kevin DELIME-CODRIN¹, Seongho CHOI¹, Keisuke HIRATA¹, Masahiro ADACHI², Makoto KIYAMA², Takashi MATSUURA², Yoshiyuki YAMAMOTO², Masaharu MATSUNAMI¹, Tsunehiro TAKEUCHI¹
¹Toyota Technological Institute, ²Sumitomo Electric Industries, Ltd.

F3-13-010 11:50–12:05

Entropy-Driven Formation of Cubic Structure GeTe
ZIHANG LIU
National Institute for Materials Science

December 13, 2019

Oral Session 8**Time** 14:00–16:10 **Room** Work-2

Chairpersons Zhigang CHEN, Teruyuki IKEDA

F3-13-K11 ▶ **Keynote** 14:00–14:25**Printed Flexible Thermoelectric Device of the Bismuth Telluride based Composite**Koji MIYAZAKI¹, Shrikant SAINI¹, Satoshi IKUBO¹,
Ajay Kumar BARANWAL², Shuzi HAYASE¹¹Kyushu Institute of Technology, ²The University of Electro-Communications**F3-13-I12** ▶ **Invited** 14:25–14:45**Thermoelectric Properties of van der Waals Materials**Taishi TAKENOBU
Nagoya University**F3-13-I13** ▶ **Invited** 14:45–15:05**New horizons in Thermoelectric Materials: inorganic-organic hybrids and machine learning for inorganic crystals**Kedar HIPPALGAONKAR

Institute of Materials Research and Engineering, A*Star

F3-13-I14 ▶ **Invited** 15:05–15:25**Thermoelectric Materials Made from Molecularly-doped Semiconducting Carbon Nanotube Networks**Yoshiyuki NONOGUCHI

Nara Institute of Science and Technology

F3-13-O15 15:25–15:40**Flexible Inorganic Thermoelectric Materials $Ag_2(S_{1-x}Se_x)$** Saurabh SINGH, Keisuke HIRATA, Takuya MATSUNAGA,
Dogyun BYEON, Masaharu MATSUNAMI,
Tsunehiro TAKEUCHI

Toyota Technological Institute

F3-13-O16 15:40–15:55**Interface Engineering for solution processed $CsSn_{1/3}$ thermoelectric film**Ajay Kumar BARANWAL¹, Shrikant SAINI², Daisuke HIROTANI³,
Tomohide YABUKI², Satoshi IKUBO³, Koji MIYAZAKI²,
Shuzi HAYASE¹¹The University of Electro-Communications, 1-5-1 Chofugaoka, Chofu, Tokyo, 182-1515, Japan, ²Kyushu Institute of Technology, 1-1 Sensuicho, Tobata, Kitakyushu, 804-8550, Japan, ³Kyushu Institute of Technology, 2-4 Hibikino, Wakamatsu, Kitakyushu, 808-0196, Japan**F3-13-O17** 15:55–16:10**Activated reactive consolidation as a new approach to fabricate highly pure intermetallic thermoelectric materials**Babak ALINEJAD, Yuma YAMAMOTO, Teruyuki IKEDA
Ibaraki University

December 13, 2019

Oral Session 9**Time** 16:30–18:45 **Room** Work-2

Chairpersons Michihiro OHTA, Yoshiyuki NONOGUCHI

F3-13-I18 ▶ **Invited** 16:30–16:50**Study on Thermoelectric Transport Properties of Tetrahedrite and Chalcopyrite based compounds**Xiaoyuan ZHOU

Chongqing University

F3-13-I19 ▶ **Invited** 16:50–17:10**Enhanced Thermoelectric Property by use of Magnetic Interaction**Naohito TSUJII, Takao MORI

National Institute for Materials Science

F3-13-O20 17:10–17:25**Substitution Effect on Thermoelectric Properties of $CePd_3$** Fumitake OGAWA, Masaharu MATSUNAMI,
Tsunehiro TAKEUCHI

Toyota Technological Institute

F3-13-O21 17:25–17:40**Thermoelectric properties of Ba substituted $SrSi_2$, $Sr_{1-x}Ba_xSi_2$** Motoharu IMAI, Shiva K. SINGH

National Institute for Materials Science

F3-13-I22 ▶ **Invited** 17:40–18:00**Could ZnO Meet the Expectations for Thermoelectric Properties - What Needs to Be Done?**Slavko BERNIK¹, Guorong LI², Emmanuel GUILMEAU³¹Jožef Stefan Institute, ²Shanghai Institute of Ceramics, Chinese Academy of Science, ³CRISMAT/ENSICAEN Laboratory**F3-13-O23** 18:00–18:15**Joint improvement of conductivity and Seebeck coefficient of atomic source assisted evaporated ZnO:Al films**Shiyong LIU

Northeastern University

F3-13-O24 18:15–18:30**Doping of CaCo- and CaMn-Ceramics improves thermoelectric conversion efficiency**Wilfried WUNDERLICH¹, Helmut T. UCHIDA²¹Tokai University, Material Science Department, ²Tokai University, Department Precision Eng.**F3-13-O25** 18:30–18:45**Thermoelectric properties of $(Pr, Nd, Sm)_{1-x}Sr_xFeO_3$ ($0.1 \leq x \leq 0.5$) oxides**Hiroshi NAKATSUGAWA¹, Shunta KAZAMA¹, Miwa SAITO²,
Yoichi OKAMOTO³¹Yokohama National University, ²Kanagawa University, ³National Defense Academy

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 11, 2019

Poster Session

Time 19:00–20:30 Room Trade-0

F3-11-P01
Magnetic coupling contributing to the enhanced thermoelectric performance of TiFe_2Sn Heusler alloys

Weihong GAO, Naohito TSUJII, Ramalingam Suresh KUMAR, Zihang LIU, Takao MORI
National Institute for Materials Science (NIMS)

F3-11-P02
Development of high performance thermoelectric thin films based on rare earth-free CoSb_3 -Skutterudite

Cédric BOURGÈS, Isao OHKUBO, Naohito TSUJII, Takao MORI
National Institute for Materials Science (NIMS)

F3-11-P03
Low thermal conductivity and promising thermoelectric performance in A_xCoSb (A = V, Nb or Ta) half-Heuslers with inherent vacancies

Jan-Willem BOS¹, Daniella FERLUCCIO¹, Robert QUINN¹, John HALPIN², Donald MACLAREN²
¹Heriot-Watt University, ²University of Glasgow

F3-11-P04
Mg-pressure-controlled Annealing for Precise Control of Mg Content and Thermoelectric Properties of Mg_2Si -based Materials

Daisuke KATO¹, Kouta IWASAKI¹, Masahito YOSHINO², Tomoaki YAMADA², Takanori NAGASAKI²
¹Toyota Boshoku Corporation, ²Department of Energy Engineering, Nagoya University

F3-11-P05
Thermoelectric Performance of n-type Mg_2Si Grown by the Vertical Bridgman Method

Yuki KAYAMA, Seiya YAMAGUCHI, Takuya KODAMA, Hiroto HAMBÄ, Daishi SHIOJIRI, Tsutomu IIDA
Tokyo University of Science

F3-11-P06
Enhanced Thermoelectric Performance through Crystal Field Engineering in Transition Metal Doped GeTe

JING SHUAI
National Institute for Materials Science

F3-11-P07
Investigation of Thermoelectric Property of In_2Te_5 and The Origin of its Low Thermal Conductivity

Wenhao ZHANG^{1,2}, Naoki SATO¹, Takao MORI^{1,2}, Kaoru KIMURA³, Kazuki TOBITA³
¹National Institute of Material Science, ²University of Tsukuba, ³University of Tokyo

F3-11-P08
Chalcogenide-based Thermoelectrics: from Glasses and Ceramics to High Temperature Refractory Rare-Earth Materials

Bhuvanesh SRINIVASAN¹, David BERTHEBAUD¹, Franck GASCOIN², Catherine BOUSSARD-PLEDEL³, Michael J. REECE⁴, Bruno BUREAU³, Takao MORI⁵
¹CNRS-Saint Gobain-NIMS, UMI 3629, Laboratory for Innovative Key Materials and Structures (LINK), National Institute for Materials Science, Tsukuba 305-0044, Japan, ²Laboratoire CRISMAT, Normandie Univ., ENSICAEN, UNICAEN, CNRS, 14000 Caen, France, ³Univ. Rennes, CNRS, ISCR – UMR 6226, F-35000 Rennes, France, ⁴Queen Mary University of London, London E1 4NS, UK, ⁵WPI International Center for Materials Nanoarchitectonics (WPI-MANA) and Center for Functional Sensor & Actuator (CFSN), National Institute for Materials Science (NIMS), Tsukuba 305-0044, Japan

F3-11-P09
First-principles Study on the Thermoelectric Performance of $\text{LaO}(\text{PbS})\text{BiS}_2$ and Its Possible Enhancement in Analogous Compounds

Keiya KUREMATSU¹, Masayuki OCHI¹, Hidetomo USUI², Kazuhiko KUROKI¹
¹Osaka University, Japan, ²Shimane University, Japan

F3-11-P10
Electron-phonon Scattering Effect on the Transport Properties of TiS_2 : A First-principles Study

Hitoshi MORI¹, Masayuki OCHI¹, Hidetomo USUI², Kazuhiko KUROKI¹
¹Osaka University, ²Shimane University

F3-11-P11
Experimental and theoretical investigations of thermoelectric properties of doped thiospinel CuCr_2S_4

Paulina KAMIŃSKA, Piotr ŚPIEWAK, Wojciech ŚWIEŹSKOWSKI
Faculty of Materials Science and Engineering, Warsaw University of Technology

F3-11-P12
Compositional Dependence Of The Thermoelectric Properties Of The Higher Boride REB_{66}

Philipp SAUERSCHNIG^{1,2}, Kantaro TSUCHIYA^{1,2}, Takaho TANAKA¹, Yuichi MICHIE¹, Jean-Baptiste VANEY¹, Takashi AIZAWA¹, Toetsu SHISHIDO³, Takao MORI^{1,2}
¹National Institute for Materials Science (NIMS), International Center for Materials Nanoarchitectonics (WPI-MANA), Namiki 1-1, Tsukuba 305-0044, Japan, ²University of Tsukuba, Graduate School of Pure and Applied Sciences, 1-1-1 Tennoudai, Tsukuba 305-8671, Japan, ³New Industry Creation Hatchery Center, Tohoku University, Sendai 980–8579, Japan

F3-11-P13
Fabrication of P-type Antimony Telluride Nanoparticles via Spontaneous Oxidation-Reduction Reaction

JUNYOUNG PARK, MASAYUKI TAKASHIRI
TOKAI UNIVERSITY

F3-11-P14

A Study on the Thermoelectric Performance and Stability of Cu₂Se-Reduced Graphene Oxide Composites

SeungHyun JIN¹, Jang-Yeul TAK², Woo Hyun NAM², YoungSoo LIM¹

¹Pukyong National University, Busan, 48547, Korea, ²Korea Institute of Ceramic Engineering and Technology, Jinju, 52851, Korea

F3-11-P15

Thermal Transport Properties of Single-Crystalline Bi₂Te₃ Nanoplate Films Determined by 3ω Method

Ryotaro MORI¹, Norimasa OGA¹, Takuya KUROKAWA¹, Saburo TANAKA², Koji MIYAZAKI³, Masayuki TAKASHIRI¹

¹Graduate School of Engineering, Tokai University, ²College of Engineering, Nihon University, ³Graduate School of Engineering, Kyushu Institute of Technology

F3-11-P16

Influence of exchange-correlation functional and potential on thermoelectric transport calculations of d⁰ perovskite oxides

Isao OHKUBO, Takao MORI

National Institute for Materials Science (NIMS)

F3-11-P17

Investigation of Interfacial Effect on Thermoelectric Properties of TiO₂ Based Layered Composite Materials

Hyoung-Won SON^{1,2}, Naoki SATO¹, Takao MORI^{1,2}

¹National Institute for Materials Science, ²University of Tsukuba

F3-11-P18

Structural Characterization and Thermoelectric Properties of Composite Materials (Ga,Al)₂O₃(ZnO)_m-ZnO:Ga,Al

Yuichi MICHIEUE¹, Hyoung-Won SON^{1,2}, Takao MORI^{1,2}

¹National Institute for Materials Science, ²University of Tsukuba

F3-11-P19

Density Functional Calculations of Thermoelectricity using Nonequilibrium Green's Function Method

Nobuhiko KOBAYASHI¹, Hirokazu TAKAKI¹, Kenji HIROSE²

¹University of Tsukuba, ²NEC

F3-11-P20

NEGF+DFT Simulation on Thermoelectric Properties of Nitrogen-doped Carbon Nanotubes

Manaho MATSUBARA

Tokyo University of Science

F3-11-P21

Molecular Dynamics Study of Thermal Conducting Behavior in Nano Multilayer Films

Masato SHIMONO¹, Hirokazu TAKAKI^{1,2},

Kazuaki KOBAYASHI¹, Nobuhiko KOBAYASHI², Kenji HIROSE³

¹National Institute for Materials Science, ²University of Tsukuba, ³Smart Energy Research Laboratories, NEC corporation

F3-11-P22

Theoretical Study on Thermoelectric Effects of Polycrystalline Bilayer Graphene

Hikaru HORII¹, Kenji SASAOKA², Takahiro YAMAMOTO^{1,2}, Hidetoshi FUKUYAMA³

¹Faculty of Engineering, Tokyo University of Science, ²RIST, Tokyo University of Science, ³Tokyo University of Science

F3-11-P23

Thermoelectric Simulation for Carbon Nanotube film

Kotaro FUJISAKI

Tokyo University of Science

F3-11-P24

Electronic Band Structure of Various TiN (ScN) dot/MgO Superlattices

Kazuaki KOBAYASHI¹, Hirokazu TAKAKI^{1,2}, Masato SHIMONO³, Nobuhiko KOBAYASHI², Kenji HIROSE⁴

¹International Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science, ²Institute of Applied Physics, University of Tsukuba, ³Research Center for Structural Materials (RCSM), National Institute for Materials Science, ⁴Smart Energy Research Laboratories, NEC corporation

F3-11-P25

MBE Fabrication of Magnesium Stannide Thin Films

Mariana LIMA^{1,2}, Takashi AIZAWA¹, Takeaki SAKURAI², Isao OHKUBO¹, Cedric BOURGES¹, Tetsuya BABA¹, Naoki SATOH¹, Takao MORI¹

¹National Institute for Materials Science, Tsukuba, 305-0044, Japan, ²University of Tsukuba, Tsukuba, 305-8577, Japan

F3-11-P26

Fabrication and evaluation of magnetic chalcopyrite thermoelectric thin films

Hong PANG¹, Cédric BOURGÈS¹, Naohito TSUJII¹, Takao MORI^{1,2}

¹National Institute for Materials Science (NIMS), ²University of Tsukuba, Graduate School of Pure and Applied Sciences

F3-11-P27

Thermoelectric Properties of Unfilled Skutterudite-Organic Hybrid Composite

Fainan FAILAMAN¹, Takao MORI^{1,2}

¹National Institute for Materials Science, ²Graduate School of Pure and Applied Sciences, University of Tsukuba

F3-11-P28

Gate-tuned Thermoelectric Performances in Aligned Conducting Polymers

Katsuya WATANABE¹, Kaito KANAHASHI², Naoya TAKEKOSHI¹, Hisaaki TANAKA¹, Hiroshi ITO¹, Hiromichi OHTA³, Taishi TAKENOBU^{1,2}

¹Nagoya University, ²Waseda University, ³Hokkaido University



F3-11-P29

Thermoelectric Properties of Carbon Nanotube with Local Distortion Deformation

Keiichiro MATSUMOTO, Takahiro YAMAMOTO
Tokyo University of Science

F3-11-P30

Ni-Based Alloy Thermoelectric Module As a Reliable Testing Reference For Power Generation

Raju CHETTY¹, Kazuo NAGASE¹, Makoto AIHARA¹,
Priyanka JOOD¹, Hiroyuki TAKAZAWA^{1,2}, Michihiro OHTA¹,
Atsushi YAMAMOTO¹

¹National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, ²Thermal Management Materials and Technology Research Association (TherMAT), Tokyo, Japan

F3-11-P31

Nanostructured PbTe- and Colusite-based Thermoelectric Power Generation: Materials and Modules

Michihiro OHTA¹, Raju CHETTY¹, Priyanka JOOD¹,
Atsushi YAMAMOTO¹, Koichiro SUEKUNI²,
Mercuri G. KANATZIDIS³

¹National Institute of Advanced Industrial Science and Technology (AIST), ²Kyushu University, ³Northwestern University and Argonne National Laboratory

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 13, 2019

Symposium F-4Synchrotron X-ray Probes for Mesoscale
Materials Science

[Organizers]

Yoshiharu SAKURAI (Japan Synchrotron Radiation Research Institute)
 Toyohiko KINOSHITA (Japan Synchrotron Radiation Research Institute)
 Di-Jing Huang (National Synchrotron Radiation Research Center)
 Veijo Honkimäki (European Synchrotron Radiation Facility)
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December 13, 2019

Oral Session 7

Time 9:30-11:40 Room Port-4

Chairperson Toyohiko KINOSHITA

Introduction: Yoshiharu Sakurai

9:30-9:40

F4-13-I01 ▶ Invited 9:40-10:10

Science Frontiers Developed by Diffraction-Limited
Synchrotron Light SourcesMakina YABASHI
RIKEN SPring-8 Center

F4-13-I02 ▶ Invited 10:10-10:40

X-ray Nano-Imaging at ESRF

Peter CLOETENS
ESRF

F4-13-I03 ▶ Invited 10:40-11:10

XTIP – A dedicated beamline for synchrotron X-ray
scanning tunneling microscopyNozomi SHIRATO, Michael FISHER, Ruben REININGER,
Volker ROSE, Saw-wai HLA
Argonne National Laboratory

F4-13-I04 ▶ Invited 11:10-11:40

X-ray studies of strong dimer phase in Li_2RuO_3 Je-Geun PARK
Seoul National University

December 13, 2019

Oral Session 8

Time 14:00-16:00 Room Port-4

Chairperson Yoshiharu SAKURAI

F4-13-I05 ▶ Invited 14:00-14:30

Phase Transition Analysis of Lithium-ion Battery
Cathodes by Using Time-Resolved X-ray Diffraction and
Improvement of Rate CapabilityYoshiharu UCHIMOTO
Kyoto University

F4-13-I06 ▶ Invited 14:30-15:00

In-situ studies of supercapacitors in operando condition
using synchrotron X-rayYan-Gu LIN
National Synchrotron Radiation Research Center

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

F4-13-I07 ▶ Invited 15:00–15:30
The Impacts of Synchrotron Characterization on Porous Absorbents and Catalysts
Shik Chi Edman TSANG
 University of Oxford

F4-13-I08 ▶ Invited 15:30–16:00
Identification of Ferrimagnetic Orbitals Preventing Jahn-Teller Distortions in $\text{Li}_x\text{Mn}_2\text{O}_4$ Cathodes
Bernardo BARBIELLINI
 LUT University (Finland)

December 13, 2019

Oral Session 9

Time 16:30–18:20 **Room** Port-4

Chairperson Di-Jing HUANG

F4-13-I09 ▶ Invited 16:30–17:00
Multi-scale 3D Imaging of Strain and Structure with Dark-Field X-Ray Microscopy
Hugh SIMONS
 Technical University of Denmark

F4-13-I10 ▶ Invited 17:00–17:30
Intragranular 3D orientation and stress mapping for bulk steel
Yujiro HAYASHI
 Toyota Central R&D Labs., Inc.

F4-13-011 17:30–17:55
Hard X-ray Ptychography and Multi-Shot Coherent Diffraction Imaging with Coherent Projection Illumination Optics
Yuki TAKAYAMA¹, Keizo FUKUDA¹, Motoki KAWASHIMA¹, Yuki AOI¹, Shotaro OKA², Hiroshi ONO², Tatsuki AKADA¹, Takumi IKEDA¹, Yasushi KAGOSHIMA¹
¹University of Hyogo, ²Toshiba Corporation

F4-13-012 17:55–18:20
High-energy x-ray nano-CT for nondestructive multiscale 3D/4D imaging
Akihisa TAKEUCHI
 JASRI / Japan

December 13, 2019

Poster Session

Time 19:00–20:30 **Room** Trade-0

F4-13-P01
Direct observation of nucleation process of magnetic vortex structure by means of time-resolved photoemission electron microscopy
Takuo OHKOCHI^{1,2}, Masaki OURA², Hitoshi OSAWA¹, Akinobu YAMAGUCHI^{2,3}, Hidenori FUJIWARA^{2,4}, Akira SEKIYAMA^{2,4}, Toyohio KINOSHITA¹
¹Japan Synchrotron Radiation Research Institute, ²RIKEN/SPRING-8, ³University of Hyogo, ⁴Osaka University

F4-13-P02
Detecting Intramolecular Dynamics of GPCRs in Living Cells Using Diffracted X-ray Blinking Technique
Masaki ISHIHARA¹, Shoko FUJIMURA², Kouhei ICHIYANAGI^{3,4}, Shunsuke NOZAWA³, Shinichi ADACHI³, Ryo FUKAYA³, Masahiro KURAMOCHI^{1,2}, Kazuhiro MIO², Yuji C SASAKI^{1,2}
¹Graduate School of Frontier Sciences, The Univ. Tokyo, ²Operand OIL, National Institute of Advanced Industrial Science and Technology, ³High Energy Accelerator Research Organization, ⁴Jichii Medical Univ.

F4-13-P03
Detector Saturation by Infrared Synchrotron Radiation and Infrared Free Electron Laser Light Sources
Yuka IKEMOTO¹, Heishun ZEN²
¹Japan Synchrotron Radiation Research Institute/Japan, ²Kyoto University

F4-13-P04
Study on mechanism and control of uniaxial magnetic anisotropy induced in the ferromagnetic/ferroelectric heterojunction using XMCD-PEEM and XPS
Akinobu YAMAGUCHI^{1,4}, Ryo NAKAMURA^{1,4}, Shunya SAEGUSA^{1,4}, Aiko NAKAO¹, Yuichi UTSUMI¹, Keisuke YAMADA², Takuo OHKOCHI^{3,4}, Toyohiko KINOSHITA³, Masaki OURA⁴
¹University of Hyogo, ²Gifu University, ³Japan Synchrotron Radiation Research Institute, ⁴RIKEN, SPRING-8 Center

F4-13-P05
X-ray Absorption Spectroscopy investigation and computer simulation of Manganese Lithium borate-based glass
Pattarpong NIJAPAI
 Suranaree University of Technology

F4-13-P06
Spin/orbital magnetization switching behaviour for CoFeB/MgO and CoFeB/Ta interface
Hiroshi SAKURAI¹, Kento HAISHI¹, Akane SHIBAYAMA¹, Kosuke SUZUKI¹, Kazushi HOSHI¹, Naruki TSUJII², Yoshiharu SAKURAI²
¹Gunma University, ²Japan Synchrotron Radiation Research Institute

F4-13-P07

Spin-Orbit Assisted Correlated Materials at High Pressure: Novel Phases and PhenomenaYang DING
HPSTAR

F4-13-P08

Non-destructive Visualization of Lithiation State in the Real Batteries using Compton Scattering ImagingKosuke SUZUKI
Gunma University

F4-13-P09

Data driven analysis of the redox factor of $\text{Li}_x\text{Ni}_{1/3}\text{Co}_{1/3}\text{Mn}_{1/3}\text{O}_2$ based on feature selection from *in-situ* XAFS/XRD data by machine-learningTakuya MORI¹, Takashi SEGI¹, Takayuki TSUBOTA¹, Lei LI², Kazushi YOKOYAMA²¹Kobelco research institute, inc., ²Hyogo Science and Technology Associations

F4-13-P10

***In-situ/Operando* Synchrotron Radiation X-ray-based Multi-analytical Measurements for Polymer Electrolyte Fuel Cells**Kotaro HIGASHI¹, Oki SEKIZAWA^{1,2}, Tomohiro SAKATA¹, Takuma KANEKO¹, Nozomu ISHIGURO³, Mizuki TADA⁴, Tomoya URUGA^{1,2}, Yasuhiro IWASAWA¹¹The University of Electro-Communications, ²Japan Synchrotron Radiation Research Institute, ³RIKEN Harima Branch, ⁴Nagoya University

F4-13-P11

Soft x-ray microbeam ARPES and High-Resolution RFA: New Photoemission Endstations at BL25SU of SPring-8Takayuki MURO
Japan Synchrotron Radiation Research Institute

F4-13-P12

Direct Observation of Anion Redox in Li-excess Oxides with Different Covalent and Ionic Characters by *operando* Soft/Hard X-ray Absorption SpectroscopyKentaro YAMAMOTO
Kyoto University

F4-13-P13

Reaction Distribution Analysis of Rechargeable Batteries using Two-dimensional X-ray ProbeYuki ORIKASA
Ritsumeikan University

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

Cluster G

Materials for Smart Systems

Symposium

- G-1 In-field Molecules for Next-generations Flexible Electronics
- G-2 **5th E&J BLS** Materials Frontier for Transparent Advanced Electronics
- G-3 Perovskite and Metal Halide Materials Based Photovoltaics and Optoelectronics
- G-4 Plasmonic Materials: from Fundamentals to Applications
- G-5 Synchrotron X-ray Characterization of Function Material Thin Films and Fine Particles

December 13, 2019

Symposium G-1

In-field Molecules for Next-generations
Flexible Electronics

[Organizers]

Tsuyoshi SEKITANI (Osaka University)
Hiroshi YAMAMOTO (Institute for Molecular Science)

December 13, 2019

Oral Session 8

Time 14:00–16:20 Room Work-3

Chairperson Hiroshi YAMAMOTO

G1-13-I01 ▶ Invited 14:00–14:20

Chiral Molecules Based Simple Spintronics

Yossi PALTIEL

The Hebrew University of Jerusalem

G1-13-I02 ▶ Invited 14:20–14:40

A hidden role of the smallness of the material in flexible devices

Fumitaka KAGAWA

University of Tokyo & RIKEN CEMS

G1-13-003 14:40–15:00

Carrier Transport in Hybrid PbS Colloidal Quantum Dot Transistors with Thiophene-Based Crosslinking Ligands

Ibuki WATANABE¹, Liming LIU¹, Satria Zulkarnaen BISRI², Ian JOHNSON³, Yasuhiro ISHIDA², Jeremy BURROUGHES³, Yoshihiro IWASA^{1,2}

¹University of Tokyo, ²RIKEN-Center for Emergent Matter Science, ³Cambridge Display Technology

G1-13-I04 ▶ Invited 15:00–15:20

Effects of Dephasing upon Quantum Dynamical Phenomena in Condensed Phase Molecular Processes

Akihito ISHIZAKI

Institute for Molecular Science, National Institutes of Natural Sciences

G1-13-I05 ▶ Invited 15:20–15:40

Gate- and strain-induced superconductivity in an organic strongly correlated transistor

Yoshitaka KAWASUGI^{1,2}, Kazuhiro SEKI³, Jiang PU⁴, Taishi TAKENOBU⁴, Seiji YUNOKI^{2,3}, Hiroshi YAMAMOTO⁵, Reizo KATO²

¹Toho University, ²RIKEN, ³RIKEN CEMS, ⁴Nagoya University, ⁵Institute for Molecular Science

G1-13-I06 ▶ Invited 15:40–16:00

Development of Organic-semiconductor injection laser

Hidekazu SHIMOTANI¹, Kanagasekaran THANGAVEL², Shun ONUKI¹, Taiki MIURA¹, Katsumi TANIGAKI^{1,2}

¹Dept. Physics, Tohoku University, ²AIMR, Tohoku University

G1-13-007 16:00–16:20

Biocompatible gel for EEG measurement with high S/N ratio

Yuki NODA, Hirokazu IIDA, Toshikazu NEZU, Tepei ARAKI, Shunsuke YOSHIMOTO, Tsuyoshi SEKITANI

Osaka University

December 13, 2019

Oral Session 9

Time 16:30–18:30 Room Work-3

Chairperson Tsuyoshi SEKITANI

G1-13-I08 ▶ Invited 16:30–16:50

Artificial Intelligence-Nanopore for Infection Control

Masateru TANIGUCHI

Osaka University

G1-13-I09 ▶ Invited 16:50–17:10

Ultra-flexible Organic photonic system

Tomoyuki YOKOTA, Takao SOMEYA

The University of Tokyo

G1-13-010 17:10–17:30

Biosignal Monitoring Systems with Bio-Conformable Organic Amplifier

Takafumi UEMURA^{1,2}, Naoko NAMBA^{1,2}, Masaya KONDO^{1,2}, Masahiro SUGIYAMA^{1,2}, Mihoko AKIYAMA¹, Shusuke YOSHIMOTO¹, Yuki NODA¹, Tepei ARAKI^{1,2}, Tsuyoshi SEKITANI^{1,2}

¹The Institute of Scientific and Industrial Research, Osaka University, ²Advanced Photonics and Biosensing Open Innovation Laboratory, AIST

G1-13-I11 ▶ Invited 17:30–17:50

Understanding and Designing High-Performance Thin-Film Transistors with Heterostructures

Chuan LIU

Sun Yat-sen University

G1-13-012 17:50–18:10

The Effect of Energy Levels on Doping Processes in Organic Semiconductors

Ross WARREN¹, Alberto PRIVITERA¹, Moritz RIEDE¹, Jenny NELSON²

¹University of Oxford, ²Imperial College London

G1-13-013 18:10–18:30

Flexible and Transparent Electrodes toward Implantable Electronics

Tepei ARAKI, Yuki NODA, Takafumi UEMURA, Shusuke YOSHIMOTO, Shintaro IZUMI, Tsuyoshi SEKITANI
Osaka University

December 13, 2019

Poster Session

Time 19:00–20:30 Room Trade-0

G1-13-P01

Role of the molecular configuration on the electronic structure of organic crystals: A combined DFT and GW study

Susumu YANAGISAWA¹, Ikutaro HAMADA²

¹University of the Ryukyus, ²Osaka University

G1-13-P02

Advancement of two-ply CNT Yarn supercapacitor properties by wet coated molybdenum oxide

Tatsuki MARUI, Yuta NISHINA, Masaki HADA, Takeshi NISHIKAWA, Yoshifumi YAMASHITA, Yasuhiko HAYASHI

Okayama University

G1-13-P03

Structure changing of residual amorphous carbon in twisted Double-Helix carbon nanotube yarns by joule heating

Shogo IEMOTO¹, Tomohiro NAKAGAWA¹, Hirotaka INOUE¹, Karthik Paneer SELVAM¹, Masaki HADA^{1,2}, Takeshi NISHIKAWA¹, Yoshifumi YAMASHITA¹, Yasuhiko HAYASHI¹

¹Okayama University, ²University of Tsukuba

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 11–13, 2019

Symposium G-2

5th E&J BLS

Materials Frontier for Transparent Advanced Electronics

[Organizers]

Yuzo SHIGESATO (Aoyama Gakuin University)
 Andreas KLEIN (Technische Universität Darmstadt)
 Nobuto OKA (Kindai University)

December 11, 2019

Oral Session 1

Time 9:00–11:30 Room Work-1

 Chairpersons Yuzo SHIGESATO, John D. PERKINS,
 Marius GRUNDMANN

 Preparation
 9:00–9:30

G2-11-K01 ▶ Keynote 9:30–10:00

Technologies for a clean and healthy Indoor environment

G. KIRIAKIDIS

IESL, FORTH and Univ. of Crete

G2-11-I02 ▶ Invited 10:00–10:30

Functionalizing transparent conducting oxides for solar cells: from disordered oxides to epitaxial perovskites

Monica MORALES MASIS, Yury SMIRNOV, Guus RIJNDERS

University of Twente. MESA+ Institute

G2-11-003 10:30–10:45

 Transparent conducting La-doped BaSnO₃: Impact of Substrate and Annealing on Optoelectrical Properties

Yury SMIRNOV, Phu Tran Phong LE, Johan E. TEN ELSHOF, Guus RIJNDERS, Monica MORALES-MASIS

MESA+ Institute for Nanotechnology, University of Twente

G2-11-I04 ▶ Invited 10:45–11:15

Developments of CuI Films as a Widegap p-Type Semiconductor.

Naoomi YAMADA

Chubu University

G2-11-005 11:15–11:30

A Study of Heterojunction Structure for In–Ga–Zn–O thin-film transistor

Daichi KORETOMO¹, Shuhei HAMADA¹, Marin MORI¹, Mamoru FURUTA^{1,2}
¹Kochi University of Technology, ²Center for Nanotechnology, Research Institute

December 11, 2019

Oral Session 2

Time 14:00–16:00 Room Work-1

 Chairpersons Monica MORALES-MASIS,
 Naoomi YAMADA

G2-11-I06 ▶ Invited 14:00–14:30

Combining Theory, Experiment and Data Analytics to Accelerate Materials Development

John PERKINS

Materials Science Center, National Renewable Energy Laboratory

G2-11-I07 ▶ Invited 14:30–15:00

Material design concept of nano-crystal embedded transparent oxide semiconductors to realize exceptional and incompatible properties for organic electronics

Nobuhiro NAKAMURA¹, Junghwan KIM², Hideo HOSONO²
¹New Product R&D Center, AGC Inc., ²Materials Research Center for Element Strategy, Tokyo Institute of Technology

G2-11-I08 ▶ Invited 15:00–15:30

Amorphous Transparent N-Type and P-Type Electronic Semiconductors for Thin Film Devices

Marius GRUNDMANN

Universität Leipzig

G2-11-I09 ▶ Invited 15:30–16:00

Effect of Metal to Semiconductor Contact Property on the Performance of Amorphous Oxide SiZnSnO Semiconductor Thin Film Transistor

Sang Yeol LEE

Cheongju University

December 11, 2019

Oral Session 3

Time 16:30–18:30 Room Work-1

Chairpersons George KIRIAKIDIS, Sang Yeol Lee

G2-11-K10 ▶ Keynote 16:30–17:00

Perspectives of Novel Applications of Ferroelectric/ Piezoelectric Thin Films for Smart Systems

Norifumi FUJIMURA

Osaka Prefecture Univ.

G2-11-I11 ▶ Invited 17:00–17:30

Impedancemetric Thick-Film Gas Sensor Based on Layered Cuprate

Youichi SHIMIZU

Kyushu Institute of Technology

G2-11-I12 ▶ Invited 17:30–18:00

Exploration of bi-functional electrode materials for oxygen reduction and oxygen evolution

Masayoshi YUASA, Miu TANAKA, Mamia YOSHIDA, Masayo SHIMIZU
Kindai University

G2-11-I13 ▶ Invited 18:00–18:30

Local Structure of Conductive Vanadate Glass and its Application to the Rechargeable Batteries

Nobuto OKA, Hajime MIYAMOTO, Ryoya SUGIMOTO, Sayaka MASUDA, Masayoshi YUASA, Tetsuaki NISHIDA
Kindai University

December 12, 2019

Oral Session 4

Time 9:00–11:30 Room Miel-2

Chairpersons Andreas KLEIN, Hiroshi YANAGI

Preparation
9:00–9:30

G2-12-I01 ▶ Invited 9:30–10:00

Solution-processed Colloidal Quantum Dot-based Infrared Photovoltaics toward Ultra-high Efficiency

Takaya KUBO
The University of Tokyo

G2-12-I02 ▶ Invited 10:00–10:30

Nanostructure and properties of solution processed oxide semiconductor films for transparent conductive electrodes

Yoshiko TSUJI, Naoya TSUTSUMI, Yuuki KOMINAMI
The University of Tokyo

G2-12-003 10:30–10:45

Numerical Simulation of Nanoparticle Network Formation in Transparent Conductive Coating

Rei TATSUMI¹, Osamu KOIKE², Yukio YAMAGUCHI², Yoshiko TSUJI¹
¹The University of Tokyo, ²Products Innovation Association

G2-12-004 10:45–11:00

Fabrication of Transparent ZnO/(CuZn)O Heterojunction Diodes by Electrochemical Deposition

Mansoureh KEIKHAEI, Masaya ICHIMURA
Nagoya Institute of Technology

G2-12-I05 ▶ Invited 11:00–11:30

Hydrogenated Indium-based and Indium-free TCOs

Luis PEREIRA, Diana GASPAS, Marco MOREIRA, Jonas DEUERMEIER, Elvira FORTUNATO, Rodrigo MARTINS CENIMAT/I3N, Faculdade de Ciências e Tecnologia, Universidade NOVA de Lisboa

December 12, 2019

Oral Session 5

Time 14:00–16:00 Room Miel-2

Chairpersons Takaya KUBO, Luis PEREIRA

G2-12-K06 ▶ Keynote 14:00–14:30

Performance and Fermi Level Limits in Oxides

Andreas KLEIN
Technische Universität Darmstadt

G2-12-I07 ▶ Invited 14:30–15:00

Electron Affinity and Ionization Potential Tuning of Amorphous Cd-In-Ga-O Films

Hiroshi YANAGI, Minseok KIM, Ryota FUJIMOTO, Kei NAKAMURA
University of Yamanashi

G2-12-I08 ▶ Invited 15:00–15:30

Effects of Mechanical and Bias Stress on Dual-gate a-IGZO-TFTs

Qun ZHANG¹, Jianwen YANG¹, Ting-Chang CHANG², Po-Yung LIAO²
¹Fudan University, ²National Sun Yat-Sen University

G2-12-I09 ▶ Invited 15:30–16:00

Amorphous IGZO Thin-Film Transistors with AlO_xH Dielectrics for Emerging Functional Applications

Shi-Jin DING
Fudan University

December 13, 2019

Oral Session 8

Time 14:00–16:00 Room Trade-1

Chairpersons Shijie WANG, Hui YE

G2-13-I01 ▶ Invited 14:00–14:30

ZnO Based Semiconductors for Excitonic Devices

Naho ITAGAKI, Kunihiro KAMATAKI, Kazunori KOGA, Masaharu SHIRATANI
Kyushu University

G2-13-I02 ▶ Invited 14:30–15:00

Functionalization of oxide-based mixed anion compound thin films

Yasushi HIROSE¹
¹The University of Tokyo, ²Kanagawa Academy of Science and Technology

G2-13-I03 ▶ Invited 15:00–15:30

Toward understanding the defect-functionality relationship in bipolar SnO thin films

Junjun JIA¹, Yuzo SHIGESATO²
¹Waseda University, ²Aoyama Gakuin University

G2-13-I04 ▶ Invited 15:30–16:00

Improved environmental stability of high-mobility In_2O_3 films fabricated at low process temperatures

Takashi KOIDA, Yuko UENO, Hajime SHIBATA
National Institute of Advanced Industrial Science and Technology (AIST)

December 13, 2019

Oral Session 9

Time 16:30–17:30 **Room** Trade-1

Chairpersons Takashi KOIDA, Yasushi HIROSE

G2-13-I05 ▶ Invited 16:30–17:00

The Dopant Localization in ZnO Materials

Shijie WANG
Institute of Materials Research and Engineering (IMRE),
A*STAR (Agency for Science, Technology, and Research)

G2-13-I06 ▶ Invited 17:00–17:30

Transparent conductive oxides: Near infrared epsilon near zero materials

Hui YE
Zhejiang University

December 12, 2019

Poster Session

Time 16:30–18:00 **Room** Trade-0

G2-12-P01

Comparison of window layers in $\text{Cu}(\text{In,Ga})\text{Se}_2$ solar cells and mini-modules

Takashi KOIDA, Yuko UENO, Jiro NISHINAGA,
Yukiko KAMIKAWA, Hirofumi HIGUCHI, Masayuki IIOKA,
Hideki TAKAHASHI, Hajime SHIBATA
National Institute of Advanced Industrial Science and Technology (AIST)

G2-12-P02

Amperometric Nitrite-Ion Sensing Properties of Perovskite-Type Oxide Based Thick-Film Electrode

Youichi SHIMIZU¹, Mikako MORIYAMA¹, Yasunari SHINODA¹,
Haruna SHIMOJI¹, Satoko TAKASE¹, Norahim IBRAHIM²
¹Kyushu Institute of Technology, ²Universiti Teknologi Malaysia

G2-12-P03

Nanocarbon Catalyst synthesized by the Solution Plasma Process for the Air-electrode of Metal-Air Battery

Ryota IMAMURA, Tomoya OKAMURA, Sayaka MASUDA,
Yui IYOKU, Ryoya SUGIMOTO, Masayoshi YUASA,
Tetsuaki NISHIDA, Nobuto OKA
Kindai University

G2-12-P04

Bifunctional Air-Electrode Catalyst composed of Ni-containing Conductive Vanadate Glass developed for Metal-Air Battery

Ryoya SUGIMOTO, Hajime MIYAMOTO, Takahisa SAKURAGI,
Sayaka MASUDA, Masayoshi YUASA, Tetsuaki NISHIDA,
Nobuto OKA
Kindai University

G2-12-P05

Carbon-doped TiO_2 Nanoparticles synthesized as the Visible-light Active Photocatalyst by Hydrothermal Method

Ryoya SUGIMOTO, Rika MIYOSHI, Sayaka MASUDA,
Tetsuaki NISHIDA, Nobuto OKA
Kindai University

G2-12-P06

Electrocatalyst for glucose oxidation and oxygen evolution using transition metal composite oxides

Masayoshi YUASA, Kouki SHIBAYAMA, Yusuke TAKIMIYA,
Shogo ASAYAMA
Kindai University

G2-12-P07

New Cathode Active Material using Vanadate Glass for High-capacity Li ion Battery

Sayaka MASUDA¹, Syunsuke MATSUSAKO¹,
Ryoya SUGIMOTO¹, Honami INADA², Hikaru HAYAKAWA²,
Tetsuaki NISHIDA¹, Nobuto OKA¹
¹Kindai University, ²MORESCO Corporation

G2-12-P08

Local Structure and Electrical Conductivity of Highly Conductive Vanadate Glass containing Tin or Indium Oxides

Sayaka MASUDA¹, Yuki FUJITA¹, Naomi YAMAGUCHI¹,
Syunsuke MATSUSAKO¹, Ryoya SUGIMOTO¹, Sachiya SHIBA²,
Shiro KUBUKI², Tetsuaki NISHIDA¹, Nobuto OKA¹
¹Kindai University, ²Tokyo Metropolitan University

G2-12-P09

Antibacterial activity of new ABC semiconductor and the effect of light irradiation

J. MIYAMOTO¹, K. ITO², K. TANAKA¹
¹Kindai University, ²Ito Research Institute Co.,Ltd.

G2-12-P10

TiO_2/WO_3 multi-layered photocatalyst with the metallic nano-particles as co-catalyst

Yuya KATO¹, Kenta TANIYAMA¹, Yuka KITAZAWA¹,
Makoto KASHIWAGI¹, Jyunjyun JIA², Shinichi NAKAMURA³,
Yuzo SHIGESATO¹
¹Graduated School of Science and Engineering, Aoyama Gakuin University, ²Faculty of Science and Engineering, Waseda University, ³Center for Instrumental Analysis, College of Science and Engineering, Aoyama Gakuin University

G2-12-P11

Electrical and Optical Properties of Nb-doped TiO₂ Films Deposited by Reactive Sputtering using Ni-Ti alloy target with impedance control systems

Nobuto OKA^{1,2}, Yuta SANNO², Junjun JIA², Yuzo SHIGESATO²
¹Kindai University, ²Aoyama Gakuin University

G2-12-P12

Solution-Processed Al-doped ZnO (AZO) Multilayer Thin-Film Transistors using Composition Controlled AZO Buffer toward Transparent Electronics

Kazuyori OURA, Keisuke TAKANO, Masatoshi KOYAMA, Toshihiko MAEMOTO, Shigehiko SASA
 Osaka Institute of Technology

G2-12-P13

Plasma Posttreatment of Transparent Conductive Electrodes

Oleg SERGEEV, Hosni MEDDEB, Hyo-Jei CHO, Kai GEHRKE, Martin VEHSE
 DLR Institute of Networked Energy Systems

G2-12-P14

Evaluation of gas barrier properties for amorphous ZnSnO_x and SiN_x films using transparent conductive oxide films

Keisuke TSUSHIMA¹, Makoto KASHIWAGI¹, Junjun JIA², Daisuke ONO³, Shigeki MATSUNAKA³, Yuzo SHIGESATO¹
¹Graduate School of Science and Engineering, Aoyama Gakuin University, ²Global Center for Science and Engineering, Faculty of Science and Engineering, ³Shibaura Mechatronics Corporation

G2-12-P15

Transparent diamond-like carbon films deposited by sputtering

Azuma NISHIZAWA¹, Nanako ISHIGURO¹, Makoto KASHIWAGI¹, Junjun JIA², Manami KUROSE³, Hironobu MACHINAGA³, Yuzo SHIGESATO¹
¹Graduate School of Science and Engineering, Aoyama Gakuin University, ²Global Center for Science and Engineering, Faculty of Science and Engineering, Waseda University, ³Core Technology Research Center, Nitto Denko Corporation

G2-12-P16

Electrical and Optical Properties of Transparent p-Type CuI Alloyed with CuBr

Yuta TANIDA, Shogo YOSHIDA, Naomi YAMADA
 University of Chubu

G2-12-P17

Zirconium oxy-sulfide: a disperse valence band, p-type transparent conductor

Angela N. FIORETTI¹, Sebastian SIOL², Christophe BALLIF¹, Mathieu BOCCARD¹, Monica MORALES-MASIS³
¹Photovoltaics and Thin Film Electronics Laboratory, Institute of Microengineering, Ecole Polytechnique Federale de Lausanne, Neuchatel, Switzerland, ²Empa–Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland, ³University of Twente, MESA+ Institute for Nanotechnology, Enschede, The Netherlands

G2-12-P18

Sputter deposition high-mobility and low-resistive amorphous In₂O₃:Sn films by using nitrogen impurities

Naho ITAGAKI, Soichiro MURAOKA, Daisuke YAMASHITA, Kunihiro KAMATAKI, Kazunori KOGA, Masaharu SHIRATANI
 Kyushu University

G2-12-P19

Homogeneous and Low-Resistivity ZnO Films by Zn Insertion

Yasuji YAMADA¹, Orkut SANCAKOGLU^{1,2}, Rei SUGIURA¹, Shuhei FUNAKI¹, Yumika YAMADA¹
¹Shimane University, ²Metallurgical and Materials Engineering, Dokuz Eylul University

G2-12-P20

Thermal Conductivity of Ti or W-doped Diamond-like carbon thin films

Takahiro SUZUKI¹, Yuichiro YAMASHITA^{1,2}, Takashi YAGI^{1,2}, Naoyuki TAKETOSHI^{1,2}, Junjun JIA³, Makoto KASHIWAGI¹, Yuzo SHIGESATO¹
¹Aoyama Gakuin University, ²National Institute of Advanced Industrial Science and Technology, ³Waseda University

G2-12-P21

Fabrication of P-doped SnO₂ thin films by pulsed laser deposition

M. FUKUMOTO, S. NAKAO, Y. HIROSE, T. HASEGAWA
 Department of Chemistry, The University of Tokyo

G2-12-P22

Crystallization Behavior of Doped Amorphous Indium Oxide Films

Shimpei IWASAKI¹, Junjun JIA², Toshihiro OKAJIMA³, Shin-ichi NAKAMURA⁴, Shingo YAMAMOTO¹, Makoto KASHIWAGI¹, Yuzo SHIGESATO¹
¹Graduate School of Science and Engineering, Aoyama Gakuin University, ²Global Center for Science and Engineering, Waseda University, ³Kyushu Synchrotron Light Research Center, ⁴Center for Instrumental Analysis, Aoyama Gakuin University

G2-12-P23

Optical properties of TiO₂, TiO_{2-x} and Nb-doped TiO₂ films analyzed by scanning ellipsometry

Yuzo SHIGESATO¹, Haruka YAMAMOTO¹, Junjun JIA², Hiroshi NISIIYAMA¹
¹Aoyama Gakuin University, ²Waseda University

G2-12-P24
Thermal conductivity of polycrystalline rutile $Ti_{1-x}Sn_xO_2$ films

Hiroki KOIZUMI¹, Takashi YAGI², Yuichiro YAMASHITA², Makoto KASHIWAGI¹, Junjun JIA³, Yuki OGUCHI¹, Naoyuki TAKETOSHI², Yuzo SHIGESATO¹

¹Graduate School of Science and Engineering, Aoyama Gakuin University, ²National Metrology Institute of Japan (NMIJ), AIST, ³Global Center for Science and Engineering, Faculty of Science and Engineering, Waseda University

G2-12-P25
Thermophysical property of Y-Mg alloy switchable mirror thin films

Hina SAITO¹, Yuichiro YAMASHITA^{1,2}, Takashi YAGI^{1,2}, Makoto KASHIWAGI¹, Junjun JIA³, Naoyuki TAKETOSHI^{1,2}, Yuzo SHIGESATO¹

¹Graduate school of Science and Engineering, Aoyama Gakuin University, ²National Metrology Institute of Japan (NMIJ), National Institute of Science and Technology (AIST), ³Global Center for Science and Engineering, Faculty of Science and Engineering, Waseda University Building 61-414

G2-12-P26
Thermophysical and optical properties of Al_2O_3 -based amorphous complex oxides films deposited by co-sputtering

Chinami ABE¹, Yuichiro YAMASHITA^{1,2}, Yukimi TANAKA², Takashi YAGI^{1,2}, Makoto KASHIWAGI¹, Junjun JIA³, Koichiro HATTORI², Naoyuki TAKETOSHI^{1,2}, Yuki OGUCHI¹, Yuzo SHIGESATO¹

¹Graduate School of Science & Engineering, Aoyama Gakuin University, ²National Metrology Institute of Japan (NMIJ), National Institute of Advanced Industrial Science and Technology (AIST), ³Global Center for Science and Engineering, Faculty of Science and Engineering, Waseda University

G2-12-P27
Development of electrochromic thin films for thermal switching devices

Koichi SAKATA¹, Takashi YAGI^{1,2}, Yuichiro YAMASHITA^{1,2}, Makoto KASHIWAGI¹, Junjun JIA³, Naoyuki TAKETOSHI^{1,2}, Yuzo SHIGESATO¹

¹Graduate school of Science and Engineering, Aoyama Gakuin University, ²National Metrology Institute of Japan (NMIJ), National Institute of Advanced Industrial Science and Technology (AIST), ³Global Center for Science and Engineering, Faculty of Science and Engineering, Waseda University

G2-12-P28
Approaches to fabricate the all-solid-state electrochromic windows

Yuki SHIRAKURA¹, Kento TERASHIMA¹, Makoto KASHIWAGI¹, Junjun JIA², Yuzo SHIGESATO¹

¹Graduate School of Science and Engineering, Aoyama Gakuin University, ²Global Center for Science and Engineering, Faculty of Science and Engineering, Waseda University

G2-12-P29
Electrochromic properties of doped IrO_2 films deposited by co-sputtering

Yuna SUGA¹, Makoto KASHIWAGI¹, Junjun JIA², Shin-ichi NAKAMURA³, Yuzo SHIGESATO¹

¹Graduate School of Science and Engineering, Aoyama Gakuin University, ²Global Center for Science and Engineering, Faculty of Science and Engineering, Waseda University, ³Center for Instrumental Analysis, College of Science and Engineering, Aoyama Gakuin University

G2-12-P30
Gas sensing properties of SnO_2 films deposited by rf magnetron sputtering

Shuhei NISHIKAWA¹, Makoto KASHIWAGI¹, Junjun JIA², Akira NAKAMURA³, Yuzo SHIGESATO¹

¹Graduate School of Science and Engineering, Aoyama Gakuin University, ²Global Center for Science and Engineering, Faculty of Science and Engineering, Waseda University, ³MITSUMI ELECTRIC CO., LTD

G2-12-P31
 H_2 gas sensing properties of Al-doped ZnO films deposited by rf magnetron sputtering

Hiroki SONE¹, Shuhei NISHIKAWA¹, Makoto KASHIWAGI¹, Junjun JIA², Akira NAKAMURA³, Yuzo SHIGESATO¹

¹Graduate School of Science and Engineering, Aoyama Gakuin University, ²Global Center for Science and Engineering, Faculty of Science and Engineering, Waseda University, ³MITSUMI ELECTRIC CO., LTD.

G2-12-P32
Deposition of stoichiometric MgF_2 films by rf magnetron sputtering

Kohei OGURA¹, Makoto KASHIWAGI¹, Junjun JIA², Hironobu MACHINAGA³, Yuzo SHIGESATO¹

¹Graduate School of Science and Engineering, Aoyama Gakuin University, ²Global Center for Science and Engineering, Faculty of Science and Engineering, Waseda University Building 61-414, ³Core Technology Research Center, Nitto Denko Corporation

G2-12-P33
Polytetrafluoroethylene (Teflon) films deposited by rf magnetron sputtering

Yuri OTANI¹, Makoto KASHIWAGI¹, Jia JUNJUN², Hironobu MACHINAGA³, Yuzo SHIGESATO¹

¹Graduate School of Science and Engineering, Aoyama Gakuin University, ²Global Center for Science and Engineering, Faculty of Science and Engineering, Waseda University Building 61-414, ³Core Technology Research Center, Nitto Denko Corporation

G2-12-P34
Self-powered Ultraviolet Photodetector Based on CuI/a-IGZO Heterojunction

Takahiro KONDO, Yuumi KONDO, Yuuta TANIDA, Naoomi YAMADA
Chubu University

G2-12-P35**Enhance Open-circuit Voltage of PbS Quantum Dot Solar Cells with Organic Surface Passivated ZnO Nanowires**

Haibin WANG
The University of Tokyo

G2-12-P36**Gd and Gd-Mg alloy films deposited by sputtering for all-solid state switchable mirror devices**

Kento TERASHIMA¹, Yuji SHITAYANAGI¹,
Makoto KASHIWAGI¹, Junjun JIA², Shin-ichi NAKAMURA³,
Yuzo SHIGESATO¹

¹Graduate school of Science of Engineering, Aoyama Gakuin University, ²Global Center for Science and Engineering, Faculty of Science and Engineering, Waseda University, ³Center for Instrumental Analysis, College of Science and Engineering, Aoyama Gakuin University

G2-12-P37**Study of MoO₃ thin film with low thermal conductivity**

Yuzuki AOKI¹, Yuichiro YAMASHITA^{1,2}, Takashi YAGI^{1,2},
Junjun JIA^{1,3}, Makoto KASHIWAGI¹, Yuki OGUCHI¹,
Naoyuki TAKETOSHI^{1,2}, Yuzo SHIGESATO¹

¹Graduate School of Science and Engineering, Aoyama Gakuin University, ²National Metrology Institute of Japan (NMIJ), AIST, ³Global Center for Science and Engineering, Faculty of Science and Engineering, Waseda University

G2-12-P38**Dielectric Function of Slightly-reduced Molybdenum Oxide (MoO_{3-x}) Films Deposited by Reactive Sputtering**

Shota CHOMEI¹, Junjun JIA², Makoto KASHIWAGI¹,
Yuzo SHIGESATO¹

¹Graduate School of Science and Engineering, Aoyama Gakuin University, 5-10-1, Fuchinobe, Sagami-hara, Kanagawa, 252-5258 Japan., ²Global Center for Science and Engineering, Faculty of Science and Engineering, Waseda University Building 61-414, 3-4-1 Okubo, Shinjuku-ku, Tokyo, 169-8555 Japan.

G2-12-P39**Piezoelectric properties of the doped ZnO and AlN_x films deposited by rf co-sputtering**

Kentaro TANAKA¹, Ryota MAEDA¹, Junjun JIA²,
Makoto KASHIWAGI¹, Yuzo SHIGESATO¹

¹Graduate School of Science and Engineering, Aoyama Gakuin University, ²Global Center for Science and Engineering, Faculty of Science and Engineering, Waseda University

G2-12-P40**Thin-Film Growth of Rocksalt-Type MgSnN₂**

Kenta MATSUURA, Naomi YAMADA
Chubu University

G2-12-P41**Growth of Halogen Doped n-Type SnS Single Crystals Using Self-Flux**

H. YANAGI¹, Y. IGUCHI¹, K. SATO¹, K. INOUE¹, I. SUZUKI²,
S. KAWANISHI²

¹University of Yamanashi, ²Tohoku University

G2-12-P42**Highly Efficient Inverted OLED with Judiciously Designed Dielectric/Metal/Dielectric Transparent Electrodes**

Li-Wei CHEN, Hao-Wu LIN
Department of Materials Science and Engineering, National Tsing Hua University

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 12–13, 2019

Symposium G-3

Perovskite and Metal Halide Materials Based
Photovoltaics and Optoelectronics

[Organizers]

Tsutomu MIYASAKA (Toin University of Yokohama)
Yoshihiko KANEMITSU (Kyoto University)
Udo BACH (Monash University)
Hyun Suk JUNG (Sungkyunkwan University)
Hao-Wu LIN (National Tsing Hua University)
Tetsuhiko MIYADERA (AIST)
Hideo OHKITA (Kyoto University)
Taiho PARK (POSTECH)
Atsushi WAKAMIYA (Kyoto University)

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Changing Life with Coating Technology

Techno Smart Corp.



TOKYO CHEMICAL INDUSTRY CO., LTD.

December 12, 2019

Oral Session 4

Time 9:00–11:30 Room Miel-1

Chairpersons Atsushi WAKAMIYA,
Masayuki CHIKAMATSU

Opening talk

9:00–9:05

G3-12-101 ▶ Invited 9:05–9:30

Progress of Lead Halide Perovskite Solar Cells and Next
Directions of Research by Compositional Engineering

Tsutomu MIYASAKA
Toin University of Yokohama

G3-12-102 ▶ Invited 9:30–9:55

Organic-Inorganic Halide Perovskites for Solar Fuel
Production

Jingshan LUO
Nankai University

G3-12-103 ▶ Invited 9:55–10:20

Up-Scaling Strategies for Metal Halide Perovskite Solar
Cells and Modules

Luis Katsuya ONO, Yabing QI
Okinawa Institute of Science and Technology Graduate
University

G3-12-104 ▶ Invited 10:20–10:45

Optical and Device Engineering in All Vacuum Deposited
Perovskite Solar Cells and Artificial Retina

Hao-Wu LIN
National Tsing Hua University

G3-12-005 10:45–11:00

Back-Contact Perovskite Solar Cells

Xiongfeng LIN, Udo BACH
Monash University

G3-12-006 11:00–11:15

Light-Induced Performance Decrease in Perovskite
Photovoltaics

Eiji KOBAYASHI, Ryoto FUNAYAMA, Akito ENDO
Kishu Giken Kogyo Co., Ltd.

G3-12-007 11:15–11:30

Effect of Low Energy Ion Irradiation on the Optical and
Electronic Properties of Perovskite Solar Cells

Hironori OGATA^{1,2,3}, Tomoaki NISHIMURA²,
Yuki FUKAZAWA¹, Masato GOCHO¹, Kazunori ITO¹,
Toshiya KOBAYASHI¹, Ryusuke UMEDA¹

¹Grad.School Sci. Technol., Hosei University, ²Res. Center
of Ion Beam Technology, Hosei University, ³Res. Center for
Micro-Nano Technol., Hosei University

December 12, 2019

Oral Session 5**Time** 14:00–16:00 **Room** Miel-1

Chairpersons Tetsuhiko MIYADERA, Takeru BESSHO

G3-12-I08 ▶ Invited 14:00–14:25

Passivation and Interface Engineering of Lead Halide Perovskite for High Performance Solar Cells

Peng GAO

Fujian Institute of Research on the Structure of Matter

G3-12-I09 ▶ Invited 14:25–14:50Surface Termination of the Solution-Processed $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskite FilmHiroyuki YOSHIDA, Abduheber MIRZEHMET

Chiba University

G3-12-I10 ▶ Invited 14:50–15:15

How to Use Synchrotron Soft X-Ray For Analysis of Perovskite Solar Cell

Seigo ITO

University of Hyogo

G3-12-011 15:15–15:30

Open-Circuit Voltage in Tin-Based Perovskite Solar Cells

Hideo OHKITA¹, Hyung Do KIM¹, Yongyoon CHO^{1,2}¹Kyoto University, ²University of New South Wales**G3-12-012** 15:30–15:45

Defect and Trap Passivation of Tin Halide Perovskite with Lewis Base

Muhammad Akmal KAMARUDIN¹, Daisuke HIROTANI², Kengo HAMADA², Kohei NISHIMURA¹, Qing SHEN¹, Taro TOYODA¹, Satoshi IIKUBO², Takashi MINEMOTO³, Kenji YOSHINO⁴, Shuzi HAYASE¹¹The University of Electro-Communications, ²Kyushu Institute of Technology, ³Ritsumeikan University, ⁴Miyazaki University**G3-12-013** 15:45–16:00

Tin-Based Perovskite Solar Cells using Precursor Materials Purified by Reducing Agents

Tomoya NAKAMURA, Shinya YAKUMARU, Jiewei LIU, Taketo HANDA, Yoshihiko KANEMITSU, Richard MURDEY, Atsushi WAKAMIYA

Institute for Chemical Research, Kyoto University

December 12, 2019

Oral Session 6**Time** 16:30–18:30 **Room** Miel-1

Chairpersons Hao-Wu LIN, Sheigo ITO

G3-12-I14 ▶ Invited 16:30–16:55

Study of Potassium Doping to the Organometal Halide Perovskite Properties and Less Hysteresis Photovoltaics with Monolithic Structure

Takeru BESSHO

The University of Tokyo

G3-12-I15 ▶ Invited 16:55–17:20

Photovoltaic Parameters in Lead-Based Perovskite Solar Cells

Hyung Do KIM, Hideo OHKITA

Kyoto University

G3-12-I16 ▶ Invited 17:20–17:45

Precise Control of Semiconductor Interfaces in Perovskite Solar Cells

Masayuki CHIKAMATSU

AIST

G3-12-017 17:45–18:00

Investigations of Crystallinity and Morphology of the Perovskite Films Fabricated by Inkjet Prints with Different Solvents

Ryoto FUNAYAMA, Eiji KOBAYASHI, Akito ENDO

Kishu Giken Kogyo Co., Ltd.

G3-12-018 18:00–18:15

Factors Determining the Vertical Orientation of Two-Dimensional Perovskites

Yuko TAKEOKA

Sophia University

G3-12-019 18:15–18:30

Highly Sensitive Photodetector Based on a Metal Complex Hybridized Structure with Perovskite Nanoparticles

Ayumi ISHII^{1,2}, Ajay K. JENA¹, Tsutomu MIYASAKA¹¹Toin University of Yokohama, ²JST, PRESTO

December 13, 2019

Oral Session 8**Time** 14:00–16:00 **Room** Miel-3

Chairpersons Hideo OHKITA, Akinori SAEKI

G3-13-I01 ▶ Invited 14:00–14:25

The Photophysics of the Disruptive Perovskites

Tze-Chien SUM

Nanyang Technological University

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

G3-13-I02 ▶ Invited 14:25–14:50
 Direct Observation of Charge Transfer at the Interface between Perovskite and PEDOT:PSS Layers
Kazuhiro MARUMOTO
 University of Tsukuba

G3-13-I03 ▶ Invited 14:50–15:15
 Light-Induced Refractive Index Changes in Metal Halide Perovskites
Hirokazu TAHARA, Taketo HANDA, Yoshihiko KANEMITSU
 Kyoto University

G3-13-004 15:15–15:30
 Ultrafast Interfacial Electron and Hole Transfer Dynamics from FAPb₃ Perovskite Quantum Dots to Electron and Hole Transport Layers
Chao DING¹, Feng LIU¹, Yaohong ZHANG¹, Daisuke HIROTANI², Xing RIN¹, Yukiko KITABATAKE³, Taro TOYODA¹, Shuzi HAYASE^{1,2}, Takashi MINEMOTO⁴, Taizo MASUDA⁵, Kenji KATAYAMA³, Qing SHEN¹
¹Faculty of Informatics and Engineering, The University of Electro-Communications, ²Graduate School of Life Science and Systems Engineering, Kyushu Institute of Technology, ³Department of Applied Chemistry, Chuo University, ⁴Department of Photonics, Ritsumeikan University, ⁵X-Frontier Division, Toyota Motor Corporation

G3-13-005 15:30–15:45
 Enhanced Near-Infrared Emission from Cs(Pb/Sn)I₃ Quantum Dots by Sodium Doping
FENG LIU, CHAO DING, Yaohong ZHANG, Qing SHEN
 The University of Electro-Communications

G3-13-006 15:45–16:00
 Non-Toxic Materials for Light-Emitting Diodes
Yu-Chiang CHAO
 National Taiwan Normal University

December 13, 2019
Oral Session 9
Time 16:30–18:40 **Room** Miel-3
 Chairpersons Yoshihiko KANEMITSU,
Tsutomi MIYASAKA

G3-13-I07 ▶ Invited 16:30–16:55
 Less-Defect Perovskite Quantum Dots: Synthesis, Optical Properties and Application to Optoelectronic Devices
Qing SHEN, Feng LIU, Yaohong ZHANG, Chao DING, Taro TOYODA, Shuzi HAYASE
 The University of Electro-Communications

G3-13-I08 ▶ Invited 16:55–17:20
 Anion Exchange Perovskite Quantum-Dots for Highly Efficient Light-Emitting-Devices
Takayuki CHIBA
 Yamagata University

G3-13-I09 ▶ Invited 17:20–17:45
 Unique Optoelectronic Properties of Pb/Sn Perovskites
Akinori SAEKI
 Osaka University

G3-13-I10 ▶ Invited 17:45–18:10
 Excitonic Properties of CH₃NH₃PbX₃ [X = I, Br, Cl] Lead Halide Perovskites Revealed by Magnetoreflectance Spectroscopy
Yasuhiro YAMADA¹, Hirofumi MINO¹, Kenichi OTO¹, Yoshihiko KANEMITSU²
¹Chiba University, ²Kyoto University

G3-13-011 18:10–18:25
 Mechanism of Efficient anti-Stokes Photoluminescence in Lead-Halide Perovskite Single Crystals
Takumi YAMADA, Yoshihiko KANEMITSU
 Institute for Chemical Research, Kyoto University

G3-13-012 18:25–18:40
 Polarization-Resolved Optical Spectroscopy in Lead Halide Perovskite CH₃NH₃PbX₃ [X = I, Br] Single Crystals
Nanako IGARASHI¹, Shunichi SAKAGUCHI¹, Kenichi OTO¹, Yoshihiko KANEMITSU², Yasuhiro YAMADA¹
¹Chiba University, ²Kyoto University

December 13, 2019
Poster Session
Time 19:00–20:30 **Room** Trade-0

G3-13-P01
 Mixed-Organic-Cation Perovskite Solar Cells Fabricated by All-Vacuum Deposition
LIN YANG, CHIEN-YU CHEN, HAO-WU LIN
 National Tsing Hua University

G3-13-P02
 High Performance Cesium Lead Halide Perovskite Quantum Dots Fabricated by Hot Spray Synthesis Technique
Bo-Wei HSU, Yung-Tang CHUANG, Hao-Wu LIN
 Materials Science and Engineering/National Tsing Hua University, Taiwan

G3-13-P03
 Metal Halide Based Artificial Synaptic Devices with Multi-Tunable-States
Wei-Chun WANG, Li-Wei CHEN, Hao-Wu LIN
 Department of Materials Science and Engineering, National Tsing Hua University

G3-13-P04
 Efficient Hole Transporting Layers for All Vacuum Processed Perovskite Solar Cell
Dan WANG, Hao-Wu LIN
 Department of Materials Science and Engineering, National Tsing Hua University

G3-13-P05

Perovskite Solar Cells: Global and Local Structure

Jintara PADCHASRI¹, Pinit KIDKHUNTHOD²,
Taras KOLODIAZHNYI³, Rattikorn YIMNIRUN⁴,
Saroj RUJIRAWAT¹

¹Suranaree University of Technology, ²Synchrotron Light
Research Institute, ³National Institute for Materials Science,
⁴Vidyasirimedhi Institute of Science and Technology

G3-13-P06

Synthesis and Properties of Hybrid Perovskite
CH₃NH₃Pb_{1-x}Cl_x Solar Cell Materials

Phitsamai KAMONPHA, Saroj RUJIRAWAT
Research Network NANOTEC-SUT on Advanced
Nanomaterials and Characterization, School of Physics,
Institute of Science, Suranaree University of Technology

G3-13-P07

Molecular Dynamics in the Hybrid Organic-Inorganic
Perovskite MAPbI₃ Probed by Muon Spin Relaxation
Technique

Akihiro KODA¹, Masatoshi HIRAISHI¹, Hirotaka OKABE¹,
Ryosuke KADONO¹, Seung-Hun LEE², Joshua J. CHOI²,
Katelyn A. DAGNALL²

¹KEK, ²University of Virginia

G3-13-P08

Influence of the Different Substrates on Spiro-OMeTAD
Layer Orientation

Hirofumi MAEKAWA
University of Hyogo

G3-13-P09

Evaluation of Thermal Durability and Radiation Resistance
of MA-Free Perovskite Solar Cells

Yuma NAGANO
University of Hyogo

G3-13-P10

Improving V_{oc} and Stabilizing Black Phase for All-
inorganic CsPbX₃ Perovskite Solar Cells

Zhanglin GUO
Toin University of Yokohama

G3-13-P11

Evaluation of Durability of Perovskite Solar Cells with
Mixed Cations and Halide Anions

Yuki FUKAZAWA, Masato GOCHO, Kazunori ITO,
Toshiya KOBAYASHI, Ryusuke UMEDA, Hironori OGATA
Grad. Sch. Sci. and Engin., Hosei Univ.

G3-13-P12

Fabrication and Properties of Inverted Perovskite Solar
Cells with Surface-Treated Nickel Oxide Films

Toshiya KOBAYASHI¹, Masato GOCHO¹, Kazunori ITO¹,
Yuki FUKAZAWA¹, Ryusuke UMEDA¹, Hironori OGATA^{1,2,3}

¹Graduate School of Science and Engineering, Hosei
University, ²Dept. Chem.Sci. and Technol., Hosei University,
³Research Center for Micro-Nano Technology, Hosei
University

G3-13-P13

Withdrawal

G3-13-P14

Transparent Organic Hole-Transporting Materials
Containing Partially Oxygen-Bridged Triphenylamine
Skeletons: Synthesis and Application for Perovskite
Solar Cells

Minh Anh TRUONG, Richard MURDEY, Atsushi WAKAMIYA
Institute for Chemical Research, Kyoto University

G3-13-P15

Observation of High-Order Harmonic Generation from
Hybrid Lead Halide Perovskites

Hideki HIRORI¹, Peiyu XIA², Yasushi SHINOHARA²,
Tomohito OTOBE³, Yasuyuki SANARI¹, Hirokazu TAHARA¹,
Nobuhisa ISHII², Jiro ITATANI², Yoshihiko KANEMITSU¹

¹Kyoto University, ²University of Tokyo, ³QST

G3-13-P16

Crystal Growth Dynamics of CH₃NH₃PbI₃ in Vacuum
Deposition Process

Tetsuhiko MIYADERA¹, Yuto AUCHI^{1,2}, Kohei YAMAMOTO¹,
Noboru OHASHI¹, Tomoyuki KOGANEZAWA³,
Hiroyuki YAGUCHI³, Yuji YOSHIDA¹, Masayuki CHIKAMATSU¹

¹National Institute of Advanced Industrial Science and
Technology, ²Saitama University, ³Japan Synchrotron
Radiation Research Institute

G3-13-P17

Anion-Exchange Blue Perovskite Quantum Dots LED
with Metal Halide

Jun SATO
Yamagata University

G3-13-P18

High Efficiency of Blue Perovskite Quantum Dots LED
Using Adamantane Additive

Shota ISHIKAWA
Yamagata University

G3-13-P19

Single Exciton Dynamics in Lead Halide Perovskite
Nanocrystals: Single Dot Spectroscopy

Yoshihiko KANEMITSU, Sojiro MASADA, Hirokazu TAHARA,
Masaki SARUYAMA, Tokuhisa KAWAWAKI, Ryota SATO,
Toshiharu TERANISHI

Institute for Chemical Research, Kyoto University

G3-13-P20

AFM Nano-Processing in Lead Halide Perovskites

Keisuke KUMAGAI¹, Shunichi SAKAGUCHI¹, Kenichi OTO¹,
Yoshihiko KANEMITSU², Yasuhiro YAMADA¹

¹Chiba University, ²Kyoto University

December 12–13, 2019

Symposium G-4

Plasmonic Materials: from Fundamentals to Applications

[Organizers]

Toshiharu TERANISHI (Kyoto University)
 Tatsuya TSUKUDA (The University of Tokyo)
 Jwa-Min NAM (Seoul National University)
 Jill E. MILLSTONE (University of Pittsburgh)
 Keiko TAWA (Kwansei Gakuin University)

December 12, 2019

Oral Session 5

Time 14:00–16:00 Room Miel-5

Chairperson Toshiharu TERANISHI

G4-12-I01 ▶ Invited 14:00–14:30

Hybrid Nanomaterials for Plasmon-Enhanced Fluorescence Spectroscopy Biosensors

Jakub DOSTALEK

AIT-Austrian Institute of Technology

G4-12-I02 ▶ Invited 14:30–15:00

Application of a Plasmonic Chip to the Brighter Fluorescence Microscopy

Keiko TAWA

Kwansei Gakuin University

G4-12-I03 ▶ Invited 15:00–15:30

Assembling Activatable Plasmonic Nanoantennas in Live Cells for Targeted SERS and Photoacoustic Imaging

Fabien PINAUD¹, Tugba KOKER¹, Nathalie TANG², Chao TIAN³, Wei ZHANG³, Xueding WANG³, Richard MARTEL²

¹University of Southern California, ²University of Montréal,

³University of Michigan

G4-12-I04 ▶ Invited 15:30–16:00

Free-Standing 2D Plasmonic Nanoassemblies

Wenlong CHENG

Monash University

December 12, 2019

Oral Session 6

Time 16:30–18:05 Room Miel-5

Chairperson Tatsuya TSUKUDA

G4-12-K05 ▶ Keynote 16:30–17:05

Enhanced Water Splitting under Modal Strong Coupling Conditions

Hiroaki MISAWA^{1,2}

¹Hokkaido University, ²National Chiao Tung University

G4-12-I06 ▶ Invited 17:05–17:35

Plasmonic Nanogap-Enhanced Raman Scattering for Biomedical Applications

Jwa-Min NAM

Seoul National University

G4-12-I07 ▶ Invited 17:35–18:05

Exotic Non-Zero Wavevector Electronic Excitation by Localized Surface Plasmon

Kei MURAKOSHI

Hokkaido University

December 13, 2019

Oral Session 8

Time 14:00–16:05 Room Work-4

Chairperson Keiko TAWA

G4-13-I01 ▶ Invited 14:00–14:30

Nanoplasmonic Materials and Structures for Bio Sensing

Hiroyuki YOSHIKAWA, Eiichi TAMIYA

Osaka University

G4-13-I02 ▶ Invited 14:30–15:00

Colloidal Plasmonic Metal Nanocrystals

Jianfang WANG

The Chinese University of Hong Kong

G4-13-I03 ▶ Invited 15:00–15:30

Imaging, Control, Impact of Chiral Plasmons

Hiromi OKAMOTO

Institute for Molecular Science

G4-13-K04 ▶ Keynote 15:30–16:05

Hot-Electron Effects in Electrically-Driven Plasmonic Nanostructures: Light, Sensing and Artificial Synapses

Alexey KRASAVIN, Anatoly ZAYATS, Yunlu JIANG,

Pan WANG, Mazhar NASIR

King's College London

December 13, 2019

Oral Session 9

Time 16:30–18:00 Room Work-4

Chairperson Jwa-Min NAM

G4-13-I05 ▶ Invited 16:30–17:00

Plasmon-Boosted Cooperative Effect in Quantum-Emitter Assembly

Hajime ISHIHARA

Osaka University

G4-13-I06 ▶ Invited 17:00–17:30

Plasmonics-Assisted Metasurfaces and Structured InterfacesYang CHEN¹, Cheng-Wei QIU²¹NUS Suzhou Research Institute, ²National University of Singapore

G4-13-I07 ▶ Invited 17:30–18:00

Alternative Plasmonic Materials for SERS and Metasurface Applications

Shangjr GWO

Academia Sinica

December 13, 2019

Poster Session

Time 19:00–20:30 Room Trade-0

G4-13-P01

Emergence of Plasmonic Behavior in Free Silver Clusters, Ag_n⁺, Studied by Photofragmentation Spectroscopy in the Size Range up to N = 70Takuya HORIO¹, Shuhei FUJIMOTO¹, Satoshi KONO¹, Masashi ARAKAWA¹, Tomokazu YASUIKE^{2,3}, Akira TERASAKI¹¹Department of Chemistry, Faculty of Science, Kyushu University, ²Department of Liberal Arts, The Open University of Japan, ³ESICB, Kyoto University

G4-13-P02

Two-photon Emission Detection of Quantum Dots with the Silver Plasmonic Chip

Yuki OMURA, Keiko TAWA

Kwansei Gakuin University

G4-13-P03

Fluorescence Detection of a Single Exosome with a Bull's Eye Plasmonic Chip under Microscope

Eri FUJIMOTO, Keiko TAWA

Kwansei Gakuin University

G4-13-P04

Evaluation of Labeled Molecules in Immunosensor with an Epi-Fluorescence Microscope

Makiko YOSHIDA, Keiko TAWA

Kwansei Gakuin University

G4-13-P05

Graphene Oxide Film Isolated Raman Spectroscopy for Subnano Particles Analysis and ApplicationYuansen TANG¹, Akiyoshi KUZUME², Kimihisa YAMAMOTO^{1,2}¹Laboratory for Chemistry and Life science, Institute of Innovative Research, Tokyo Institute of Technology, ²JST-ERATO in Tokyo Institute of Technology

G4-13-P06

Stabilization of Copper Nanoparticle for Novel Red OverglazeShohei SHIOMI¹, Yuki OKAZAKI¹, Hajime TAGUCHI¹, Eiichiro MATSUBARA²¹Kyoto Municipal Institute of Industrial Technology and Culture, ²Kyoto University

G4-13-P07

Toroidal Plasmons of Multilayer Metal Nanorings

T. Thuy TRINH, Toshiharu TERANISHI

Institute for Chemical Research, Kyoto University

G4-13-P08

Microspectroscopic Analysis of a Fluorescence Enhancement by the Plasmonic Chip

Hinako CHIDA, Keiko TAWA

Kwansei Gakuin University

G4-13-P09

Extraordinary Field Enhancement at TiO₂ Nanogap: Plasmon-Free Enhancement up to 2000-Fold and Its High ReproducibilityKaito HANATANI¹, Masanori SAKAMOTO¹, Kumi YOSHIHARA¹, Ken-ichi SAITOW²¹Department of Chemistry, Graduate school of science, Hiroshima Univ., ²N-BARD, Hiroshima Univ.

G4-13-P10

Localized Surface Plasmon Resonance of Ultrathin Gold NanorodsRyo TAKAHATA^{1,2}, Tatsuya TSUKUDA¹¹The University of Tokyo, ²Kyoto University

G4-13-P11

Colloidal Au Nanocups with Magnetic Plasmon Resonance

Han ZHANG, Jianfang WANG

The Chinese University of Hong Kong

G4-13-P12

Synergistically Improvement of the Plasmonic Enhancement Effect Using by Carrier-Selective Blocking LayerTokuhisa KAWAWAKI¹, Tatsuo NAKAGAWA³, Masanori SAKAMOTO², Toshiharu TERANISHI²¹Department of Applied Chemistry, Faculty of Science, Tokyo University of Science, ²Institute for Chemical Research, Kyoto University, ³Optical Instruments Division, Unisoku Co., Ltd.

G4-13-P13

Coloration of Gold Leaf using Gold NanoparticlesKazuhiro SHIMADA¹, Kimihiro NUMANO², Shinya MAENOSONO²¹Industrial Research Institute of Ishikawa, ²School of Materials Science, Japan Advanced Institute of Science and Technology

G4-13-P14
Theory of Optical Response Measurement of Single Nanoparticles by Photoinduced Force Microscopy

Hidemasa YAMANE¹, Nobuhiko YOKOSHI¹, Hajime ISHIHARA^{1,2}

¹Osaka Prefecture University, ²Osaka University

G4-13-P15
Chiral Optical Near-Fields Created by Plasmonic Nanostructures

Shun HASHIYADA¹, Tetsuya NARUSHIMA², Hiromi OKAMOTO²

¹Innovative Photon Manipulation Research Team, RIKEN Center for Advanced Photonics, ²Institute for Molecular Science and The Graduate University for Advanced Studies (Sokendai)

G4-13-P16
Two-Photon Fluorescence of Rhodamine 6G and Eu-diketonate Complex Enhanced by Silver Nanoprisms

Janice B. RABOR, Koki KAWAMURA, Yasuro NIIDOME
Kagoshima University

G4-13-P17
Developments of Nano-Structured Semi-Conductor-Assisted (NASSCA) Optical Tweezers toward Manipulation of Plasmonic Nanoparticles

Sawa KOMOTO¹, Tatsuya SHOJI¹, Saulius JUODKAZIS², Yasuyuki TSUBOI¹

¹Osaka City University, ²Swinburne University of Technology

G4-13-P18
Size Selective Optical Trapping of Polystyrene Nanoparticles using Plasmonic and Non-plasmonic nanostructures

Sayaka HASHIMOTO¹, Tatsuya SHOJI¹, Saulius JUODKAZIS², Yasuyuki TSUBOI¹

¹Osaka City University, ²Swinburne University of Technology

G4-13-P19
Ligand Effect of Porphyrin-Protected Gold Clusters and Nanoparticles in the Electrochemical Hydrogen Evolution Reaction

Daichi EGUCHI¹, Masanori SAKAMOTO², Toshiharu TERANISHI²

¹Kwansei Gakuin University, ²Institute for Chemical Research, Kyoto University

G4-13-P20
Promoting Electrocatalytic Oxygen Reduction Reaction of Octahedral Au@Pt Core-Shell Nanoparticles by Surface Plasmon Excitation

Tatsuya KAMEYAMA, Kentaro SATO, Tsukasa TORIMOTO
Nagoya University

G4-13-P21
Plasmonic and Non-Plasmonic Optical Trapping of Thermoresponsive Polymer Chains Using Nanostructured Solid Substrates

Tatsuya NAGAI¹, Tatsuya SHOJI¹, Denver LINKLATER², Saulius JUODKAZIS², Yasuyuki TSUBOI¹

¹Osaka City University, ²Swinburne University of Technology

G4-13-P22
Novel Latex Particles Decorated with Au or Pt Nanoparticles as Probes for Lateral Flow Immunochromatographic Strips with Enhanced Sensitivity

Yasufumi MATSUMURA¹, Yasushi ENOMOTO¹, Mari TAKAHASHI², Shinya MAENOSONO²

¹NIPPON STEEL Chemical & Material Co.,Ltd., ²School of Materials Science, JAIST

G4-13-P23
A Study of Colorimetric Biosensor by use of Plasmonic Full Color

Yuichiro MIYAKE¹, Sou RYUZAKI¹, Yusuke ARIMA¹, Koichi OKAMOTO², Kaoru TAMADA¹

¹Kyushu University, ²Osaka Prefecture University

G4-13-P24
Transferrin-Modified Magnetic-Plasmonic Hybrid Nanoparticles Designed for Organelle Targeting

Mari TAKAHASHI, Youren WANG, Kazuaki MATSUMURA, Shinya MAENOSONO

School of Materials Science Japan Advanced Institute of Science and Technology

G4-13-P25
Plasmonic Chiroptical Responses of 3D Continuous Chiral Nanoparticles

Hyo-Yong AHN^{1,2}, Shun HASHIYADA¹, Tetsuya NARUSHIMA^{1,3}, Hye-Eun LEE², Ki Tae NAM², Hiromi OKAMOTO^{1,3}

¹Institute for Molecular Science, Okazaki, Japan, ²Seoul National University, Seoul, Korea, ³The Graduate University for Advanced Studies, Okazaki, Japan

G4-13-P26
Chemical Induced Permittivity-Change (CIP) Effects for Metal Nanoparticles

S. RYUZAKI^{1,2}, N. SAITO¹, Y. NOGUCHI³, Y. TSUJI¹, K. YOSHIZAWA¹, K. OKAMOTO⁴, K. TAMADA¹

¹Kyushu University, ²PRESTO, JST, ³Meiji University, ⁴Osaka Prefecture University

G4-13-P27
Coherent Acoustic Phonon Vibration and Phonon Beat in Gold Nanopolyhedrons

Li WANG¹, Shohei TAKEDA¹, Masanori SAKAMOTO², Toshiharu TERANISHI², Naoto TAMAI¹

¹Kwansei Gakuin University, ²Institute for Chemical Research, Kyoto University

G4-13-P28**Isotopic Hydrogen Evolution Reactions Driven by Plasmon-Induced Charge Transfer**

Hiro MINAMIMOTO, Daiki SATO, Kei MURAKOSHI
Hokkaido University

G4-13-P29**Electrochemical Control of the Strong Coupling State between Dye Molecules and Surface Lattice Resonance**

Shunpei OIKAWA, Hiro MINAMIMOTO, Kei MURAKOSHI
Hokkaido University

G4-13-P30**Control of Emission photon Statistics of Single Quantum Dots Using Plasmonic Nanostructures**

Yoshua Albert DARMAWAN, Takaki NAKAGAWA,
Mitsuaki YAMAUCHI, Sadahiro MASUO
Kwansei Gakuin University

G4-13-P31**Near-Field Optical Imaging of Plasmon Modes Induced in Two-Dimensional Gold Nanoplates**

Keisuke IMAEDA, Takuya MATSUURA, Seiju HASEGAWA,
Kohei IMURA
Waseda University

G4-13-P32**Ionization Assisting Ability of Plasmonic Particles and Magnetic Nanoparticles as Matrices for Mass Spectrometry**

Kota AOKI, Sota HAMADA, Shota MORIMOTO,
Kouhei KANDA, Akito OSHIMA, Yuko ICHIYANAGI
Yokohama National University

G4-13-P33**Plasmon Enhanced Molecular Fluorescence Near Single Gold Mesoplates**

Seiju HASEGAWA, Keisuke IMAEDA, Kohei IMURA
Waseda University

G4-13-P34**Optical Coupling of Short-range Ordered Nanopores Through Surface Plasmons**

Dung Thi VU, Takumi SANNOMIYA
Tokyo Institute of Technology

G4-13-P35**Wide Controllability of Localized Surface Plasmon Resonance Wavelength for Au-Ag Nanorings from Visible to Near-infrared Light Region**

Kosuke SASAMOTO, Tatsuya KAMEYAMA,
Tsukasa TORIMOTO
Graduate School of Engineering, Nagoya University

G4-13-P36**Alchemy for Plasmonics: Coinage Metal-Free Visible-Plasmonic Nanoalloys**

Ryota SATO¹, Kenji IIDA², Tokuhisa KAWAWAKI³,
Katsuyuki NOBUSADA², Toshiharu TERANISHI¹
¹Kyoto University, ²Institute for Molecular Science, ³Tokyo University of Science

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 13, 2019

Symposium G-5

Synchrotron X-ray Characterization of Function Material Thin Films and Fine Particles

[Organizers]

Ichiro HIROSAWA (Japan Synchrotron Radiation Research Institute)
 Toyohiko KINOSHITA (Japan Synchrotron Radiation Research Institute)
 Jong Hyun Kim (Pohang Accelerator Laboratory)
 Anna Stenstam (CR Competence)

[Sponsors]



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December 13, 2019

Oral Session 8

Time 14:00-16:10 Room Work-8

Chairperson Norimichi SANO

Introduction: Ichiro Hirose

14:00-14:05

G5-13-I01 ▶ Invited 14:05-14:25

Time Resolved X-ray Reflectivity Study of the Early Process of Iron Passivation

Yusuke WAKABAYASHI
 Tohoku University

G5-13-002 14:25-14:40

M12 approach to modeling atmospheric corrosion of steel by using synchrotron measurement

Takahiro OZAWA¹, Shintaro YAMAMOTO¹, Takuya MORI², Mitsutoshi YOKOMIZO², Yoshimasa URUSHIHARA³, Masashi YOSHIMURA³, Kazushi YOKOYAMA³
¹Kobe Steel, Ltd., ²KOBELCO research institute, ³University of Hyogo

G5-13-I03 ▶ Invited 14:40-15:00

Synchrotron Structure Analysis on Amorphous Oxide Semiconductors

Akihiko FUJIWARA
 Kwansai Gakuin University

G5-13-I04 ▶ Invited 15:00-15:20

In-Situ Observation of Thin Film Growth of Organic Semiconductors by 2D- X-ray Diffraction

Noriyuki YOSHIMOTO¹, Daiki KUZUHARA¹, Mamoru KIKUCHI¹, Tomoyuki KOGANEZAWA², Ichiro HIROSAWA²
¹Iwate University, ²JASRI

G5-13-I05 ▶ Invited 15:20-15:40

Characterization of Local Strain in Group-IV Semiconductor Nanostructures using Microdiffraction

Osamu NAKATSUKA
 Nagoya University

G5-13-006 15:40-15:55

Investigation of Phonon Dispersion Curve for Silicon Germanium Alloy by Using Inelastic X-ray Scattering

Ryo YOKOGAWA^{1,2}, Kazutoshi YOSHIOKA¹, Haruki TAKEUCHI¹, Yasutomo ARAI³, Hiroshi UCHIYAMA⁵, Atsushi OGURA¹
¹Meiji University, ²JSPS Research Fellow DC, ³JAXA, ⁴Toshiba Memory Corporation, ⁵JASRI

G5-13-007

15:55–16:10

Synchrotron Radiation X-ray Diffraction Study on Co₅₀Pt₅₀ Thin Films Annealed by Rapid Thermal Annealing

Ryo TOYAMA¹, Shiro KAWACHI^{1,2}, Soshi IIMURA¹, Jun-ichi YAMAURA^{1,2}, Youichi MURAKAMI^{1,2}, Hideo HOSONO¹, Yutaka MAJIMA¹

¹Tokyo Institute of Technology, ²KEK

December 13, 2019

Oral Session 9

Time 16:30–18:20 **Room** Work-8

Chairperson Takeshi WATANABE

G5-13-I08

▶ Invited

16:30–16:50

Synchrotron x-ray characterization of highly functionalized catalysts and devices for a hydrogen society

Hideto IMAI
NISSAN ARC Ltd.

G5-13-I09

▶ Invited

16:50–17:10

Spectroscopy Measurements in Home lab Environment: HAXPES and Ambient Pressure for the Future

Susanna ERIKSSON
Scienta Omicron

G5-13-I10

▶ Invited

17:10–17:30

Operando and in-situ Analyses of Materials for Polymer Electrolyte Fuel Cells

Junji INUKAI
University of Yamanashi

G5-13-I11

▶ Invited

17:30–17:50

In situ X-ray Raman Scattering Spectroscopy of a Graphite Electrode for Li-ion Batteries

Takamasa NONAKA, Hiroyuki KAWAURA, Yoshinari MAKIMURA, Yusaku F. NISHIMURA, Kazuhiko DOHMAE
Toyota Central R&D Labs., Inc.

G5-13-012

17:50–18:05

Distinct Electronic Character and Selective Control of Localized vs. Delocalized Carriers at (001) Surface of Anatase TiO₂

Jun FUJII¹, Chiara BIGI^{1,2}
¹CNR-IOM, ²Università degli Studi di Milano

G5-13-013

18:05–18:20

Synchrotron-based X-ray Absorptions Studies Diamond-like Carbon Films by Ar/CH₄ flow rates Dependence of PECVD Technique

Thanun CHUNJAEMSRI¹, Narong CHANLEK^{1,2}, Pinit KIDKHUNTHOD^{1,2}, Hideki NAKAJIMA², Sarayut TUNMEE², Rattikorn YIMNIRUN³, Saroj RUJIRAWAT¹

¹Suranaree University of Technology, ²Synchrotron Light Research Institute, ³Vidyasirimedhi Institute of Science and Technology

December 13, 2019

Poster Session

Time 19:00–20:30 **Room** Trade-0

G5-13-P01

Transmission Soft X-Ray Absorption Spectroscopy on Thin Films for Li-Ion Battery

Koji HORIBA¹, Miho KITAMURA¹, Kazunori NISHIO², Ryota SHIMIZU², Taro HITOSUGI¹, Hiroshi KUMIGASHIRA^{1,3}
¹Photon Factory, Institute of Materials Structure Science, High Energy Accelerator Research Organization, ²School of Materials and Chemical Technology, Tokyo Institute of Technology, ³Institute of Multidisciplinary Research for Advanced Materials, Tohoku University

G5-13-P02

Laboratory Scale Hard X-ray Photoelectron Spectroscopy in Comparison with SPRing-8

Tappei NISHIHARA¹, Hiroki KANAI¹, Takefumi KAMIOKA¹, Toshiro OKAWA², Ichiro HIROSAWA³, Satoshi YASUNO³, Koji USUDA⁴
¹Meiji University, ²Scientaomicon, ³JASRI, ⁴Toshiba Memori Co.

G5-13-P03

Characterization of Au/Ni Ohmic Contact on p-GaN Using Hard X-ray Photoelectron Spectroscopy and 2D-X-ray Diffraction

Satoshi YASUNO¹, Tomoyuki KOGANEZAWA¹, So KUROYANAGI², Naotaka IWATA²
¹Japan Synchrotron Radiation Research Institute, ²Toyota Technological Institute

G5-13-P04

Development of instrumentation for operando hard X-ray photoemission spectroscopy of organic thin film transistors

Takeshi WATANABE¹, Satoshi YASUNO¹, Noriyuki YOSHIMOTO², Ichiro HIROSAWA¹
¹Japan Synchrotron Radiation Research Institute, ²Iwate University

G5-13-P05

Quantitative analysis of energy loss process for the core level intensities in Hard X-ray Photoemission

Takehisa KONISHI¹, Shigenori UEDA², Toyohiko KINOSHITA³
¹Department of Chemistry, Chiba University, ²Synchrotron X-ray Group, National Institute for Materials Science (NIMS), ³Japan Synchrotron Radiation Research Institute (JASRI)

G5-13-P06

XPS and Reflectivity Investigation of Silicon Oxide Thin Film Sputtered on Aluminum Layer

Ekachai CHONGSEREECHAROEN
Suranaree University of Technology

G5-13-P07**Non-distractive Characterization of Thin Amorphous Film on Substrate by Grazing-incidence X-ray Scattering**Ichiro HIROSAWA, Satoshi YASUNO

Japan Synchrotron Radiation Research Institute

G5-13-P08**Thickness-Dependent Properties of Ultrathin Diamond-like Carbon Films Prepared by Filtered Cathodic Vacuum Arc.**Warintorn CHATARAT

Suranaree University of Technology

G5-13-P09**Stabilization of Charge Order Structure in Stoichiometric YbFe_2O_4** Kosuke FUJIWARA^{1,2}, Pierre-Eymeric JANOLIN³, Stéphane GRENIER⁴, Jean-Michel KIAT³, Naoshi IKEDA²¹Japan Synchrotron Radiation Research Institute(JASRI),²Graduate School of Natural Science and Technology,Okayama University, ³CentraleSupélec, ⁴Institut NÉEL**G5-13-P10****Evaluation of Temperature and Ge Concentration Dependence of EXAFS Oscillations in SiGe thin Films**Kazutoshi YOSHIOKA¹, Ryo YOKOGAWA^{1,2}, Yuki TAKAHASHI¹, Haruki TAKEUCHI¹, Ichiro HIROSAWA³, Takeshi WATANABE³, Atsushi OGURA¹¹Meiji University, ²JSPS Research Fellow DC, ³Japan Synchrotron Radiation Research Institute (JASRI)

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

Cluster H

Green Technology and Processing

Symposium

- H-1 Advanced Water Science and Technology
- H-2 Plasma-Based Synthesis, Processing and Characterization of Materials for Energy and Environment
- H-3 **5th E&J BLS** Advanced Functional Oxides: Processing, Characterization and Devices
- H-4 A3+ Lead-free Piezoelectric Materials and Applications
- H-5 Intelligent Material Processes with Low Environmental Load and Energy Consumption

December 11–12, 2019

Symposium H-1

Advanced Water Science and Technology

[Organizers]

Osamu TAKAI (Kanto Gakuin University)
Katsuya TESHIMA (Shinshu University)

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December 11, 2019

Oral Session 1

Time 9:00–11:45 Room Miel-3

Chairpersons Katsuya TESHIMA, Norifumi ISU,
Osamu TAKAI

Opening Talk: Osamu Takai

9:00–9:05

H1-11-I01 ▶ Invited 9:05–9:25

Progress in Solution Plasma Research

Osamu TAKAI

Materials and Surface Engineering Research Institute,
Kanto Gakuin University

H1-11-I02 ▶ Invited 9:25–9:45

Antibacterial Ceramics and Uncertainty of Antibacterial
Test Method

Norifumi ISU

LIXIL Corp.

H1-11-I03 ▶ Invited 9:45–10:05

H₂O₂ Synthesis Using 3D Integrated Micro Solution
Plasma and Improvement of Its Efficiency by Combining
with Ion Exchange Resin

Tatsuru SHIRAFUJI, Shoma MIYAMOTO, Jun-Seok OH

Osaka City University

H1-11-I04 ▶ Invited 10:05–10:25

Atmospheric-pressure Plasma Reactor Generated
Plasma-activated Water

Jun-Seok OH, Yusuke SASAKI, Soshi IMAI, Tatsuru SHIRAFUJI
Osaka City University

H1-11-I05 ▶ Invited 10:25–10:45

Selective Permeation of Solutes through Microporous
Polymer Membranes prepared by Chemical Vapor
Deposition

Mutsumi KIMURA

Shinshu University

H1-11-K06 ▶ Keynote 10:45–11:15

A Perspective on Heterogeneous Integrated Edge
Devices for Internet of Things (IOT) to Enable Green
Energy Water Nexus

G.P. LI

University of California, Irvine

H1-11-007 11:15–11:30

Solution Plasma Process: a novel method for wastewater treatmentMONGKOL TIPLOOK¹, HYMIN KIM², SANGWOO CHAE^{1,4}, PHUWADEJ PORNAROONTHAM^{1,4}, NAGAIHIRO SAITO^{1,3,4,5}¹Department of Chemical Systems Engineering, Graduate School of Engineering, Nagoya University, ²LG Chem, Ltd., ³Conjoint Research Laboratory in Nagoya University, Shinshu University, ⁴Japan Science and Technology Corporation (JST), Open Innovation Platform with Enterprises, Research Institute and Academia (OPERA), ⁵Japan Science and Technology Corporation (JST), Strategic International Collaborative Research Program (SICORP)

H1-11-008 11:30–11:45

The Hardness of Single Crystal Sapphire under Controlled High TemperatureToshiro OKAWA^{1,2}, Katsuhiko TASHIRO^{2,3}, Hideo HONMA^{2,3}, Osamu TAKAI^{2,3}¹ScientaOmicron Inc., ²Materials & Surface Engineering Research Institute, Kanto Gakuin University, ³Research Advancement and Management Organization, Kanto Gakuin University

December 11, 2019

Oral Session 3

Time 16:30–18:30 Room Miel-3

Chairpersons Chiaki TERASHIMA, Masahiro MOTOSUKE

H1-11-I09 ▶ Invited 16:30–16:50

Blood Flow Characterization for Advanced DiagnosticsMasahiro MOTOSUKE
Tokyo University of Science

H1-11-I10 ▶ Invited 16:50–17:10

Development of Polymer Nano-Film Synthesized on Self-Assembled Phospholipid Layer Fabricated by Plasma-Assisted MethodShin-ichi KONDO¹, Yasushi SASAI¹, Naoki DOI¹, Yukinori YAMAUCHI², Masayuki KUZUYA³¹Gifu Pharmaceutical University, ²College of Pharmaceutical Sciences, Matsuyama University, ³Faculty of Human Welfare, Chubu Gakuin University

H1-11-I11 ▶ Invited 17:10–17:30

Preparation of Corrosion Resistant Composite Hydroxide Films on Magnesium Alloys by Steam Coating

Takahiro ISHIZAKI, Tomohiro MIYASHITA, Momo INAMURA, Yuma NAGAHIMA

Shibaura Institute of Technology

H1-11-I12 ▶ Invited 17:30–17:50

A Superhydrophilic Property and Antireflectivity of a Hierarchical Nanoporous Layer GlassTakuya FUJIMA^{1,2}, Erika TABATA¹, Takumi ITO¹, Yuki USHIODA¹¹Department of Mechanical Engineering, Tokyo City University, ²Advanced Research Laboratories, Tokyo City University

H1-11-I13 ▶ Invited 17:50–18:10

Photofuel Cells Using Porous Titania AnodesHiromasa NISHIKIORI
Shinshu University

H1-11-I14 ▶ Invited 18:10–18:30

Direct Pattern Plating on UV-modified Resins by Electroless Plating MethodYoshio HORIUUCHI¹, Michinori TAKAGI², Mikio USHIYAMA³, Manabu YASUI³, Mitsuhiro WATANABE¹, Osamu TAKAI¹, Hideo HONMA¹¹Materials and Surface Engineering Research Institute, Kanto Gakuin University, ²Azuma, ³Kanagawa Institute of Industrial Science and Technology

December 12, 2019

Oral Session 4

Time 9:00–12:25 Room Miel-3

Chairpersons Tomonaga UENO, Tomohito SUDARE, Yosuke KAGESHIMA

H1-12-I01 ▶ Invited 9:00–9:20

Enhanced Photoelectrochemical Water Reduction on the Photocathode Modified with Pt-Loaded TiO₂ NanoparticlesYosuke KAGESHIMA
Shinshu University

H1-12-I02 ▶ Invited 9:20–9:40

Tunable Heteroatom-doped Carbon as Economic and Efficient Oxygen Evolution Reaction Catalysts in Water ElectrolysisOi Lun Helena LI, Wenwei YAO, Jihoon KIM
Pusan National University

H1-12-I03 ▶ Invited 9:40–10:00

Solar light-driven Photocatalysis/Photoelectrocatalysis Water Pollutant Treatment: Pathways to Circular EconomySudhagar PITCHAIMUTHU
Swansea University

H1-12-I04 ▶ Invited 10:00–10:20

High Speed Nickel plating using Watt Nickel plating solutionYasushi UMEDA
Kanto Gakuin University Materials & Surface Engineering Research Institute

H1-12-I05 ▶ Invited 10:20–10:40

Efficient water purification by synergetic effect on mesoporous TiO₂/BDD hybrid electrodeNorihiko SUZUKI¹, Akihiro OKAZAKI², Aiga HARA¹, Yui HIRANO¹, Yukihiko NAKABAYASHI¹, Nitish ROY¹, Haruo KURIYAMA², Izumi SERIZAWA², Chiaki TERASHIMA¹, Kazuya NAKATA¹, Ken-ichi KATSUMATA¹, Takeshi KONDO¹, Makoto YUASA¹, Akira FUJISHIMA¹¹Tokyo University of Science, ²ORC Manufacturing Co., Ltd

H1-12-I06 ▶ Invited 10:40–11:00

Deposition of Copper on Glass Substrates Using a Titanium Oxide Adhesion Layer

Christopher E. J. CORDONIER, Kyohei OKABE, Hideo HONMA
Kanto Gakuin University, Materials & Surface Engineering Research Institute

H1-12-I07 ▶ Invited 11:00–11:20

Adsorption-induced Electrochromic Phenomenon of Indium-nitride Films in Aqueous Solutions

Yasushi INOUE
Chiba Institute of Technology

H1-12-I08 ▶ Invited 11:20–11:40

Aqueous Solution-based Self-Assembly of 3D Carbon Nanotube Network For High Energy Density Lithium Ion Batteries

Nobuyuki ZETTSU, Dae-wook KIM, Hye-min KIM, Katsuya TESHIMA
Shinshu University

H1-12-009 11:40–11:55

Fabrication of Three-Dimensional Structure by High-Speed Copper Sulfate Plating

Yohei SUZUKI, Yasushi UMEDA, C.E.J CORDONIER, Hideo HONMA, Osamu TAKAI, Joo-Hyong NOH
Kanto Gakuin University

H1-12-010 11:55–12:10

Surface Modification of Di-Electric Material using Photo Pretreatment

JONG-YOUNG PARK^{1,2,3}, YOUNG-JAE KIM^{2,3}, HIDEO HONMA^{1,2,3}, JOO-HYONG NOH^{1,2,3}
¹Department of Materials and Surface Engineering, Graduate School of Engineering, Kanto Gakuin University, ²Materials and Surface Engineering Research Institute, Kanto Gakuin University, ³Daeduck Electronics Co. Ltd

H1-12-011 12:10–12:25

Intelligent manipulation and transportation of water in the magnetic tubular microactuators(MTMAs)

Wenwei LEI^{1,2}, Norihiro SUZUKI¹, Chiaki TERASHIMA¹, Akira FUJISHIMA¹, Lei JIANG²
¹Tokyo University of Science, ²Beihang University

December 12, 2019

Oral Session 5
Time 14:00–16:00 **Room** Miel-3

Chairpersons Tatsuru SHIRAFUJI, Jun-Seok OH

H1-12-I12 ▶ Invited 14:00–14:20

Flash Lamp Annealing Method for Plated Films on Resin Substrates

Joo-Hyong NOH^{1,2}, YUSUKE MIYAZEKI^{1,3}, JONG-YOUNG PARK^{1,2,4}, YOSHIO HORIUCHI¹, TARO ARAKAWA³, OSAMU TAKAI¹, HIDEO HONMA^{1,2}
¹Materials and Surface Engineering Research Institute, Kanto Gakuin University, ²Graduate School of Engineering, Kanto Gakuin University, ³Graduate School of Engineering, Yokohama National University, ⁴Daeduck Electronics Co. Ltd.

H1-12-I13 ▶ Invited 14:20–14:40

Formation of High Adhesion Metal Films on ABS Resin by Closed Systemized Fine Bubble Low Ozonated Water

Katsuhiko TASHIRO
Kanto Gakuin University

H1-12-I14 ▶ Invited 14:40–15:00

Paper-based Biofuel Cell for Next Generation Energy Harvester and Wearable Healthcare Device

Isao SHITANDA
Tokyo University of Science

H1-12-I15 ▶ Invited 15:00–15:20

Green and sustainable anticorrosive coating technology using steam on Aluminum alloys

Ai SERIZAWA, Kohei WATANABE, Takeo KOIKE, So Yoon LEE, Takahiro ISHIZAKI
Shibaura Institute of Technology

H1-12-I16 ▶ Invited 15:20–15:40

Water Freezing Behavior on Aluminum Alloy Modified with Various Functional Groups

Junko HIEDA
Nagoya University

H1-12-I17 ▶ Invited 15:40–16:00

Transformation of bulk alloys to metal-organic and ceramic nanowires

Kostiantyn TURCHENIUK, Fujia WANG, Shunrui LUO, Danni LEI, Jim BENSON, Alexandre MAGASINSKY, Gleb YUSHIN, Ting ZHU, Baolin WANG
Georgia Institute of Technology

December 12, 2019

Oral Session 6**Time** 16:30–18:40 **Room** Miel-3Chairpersons Nobuyuki ZETTSU, Takahiro ISHIZAKI,
Ai SERIZAWA**H1-12-K18** ▶ **Keynote** 16:30–17:00**Engineering Perspectives of Water and Ionic Solution
Constrained at Interfacial Nanostructures**Katsumi KANEKO
Shinshu University**H1-12-I19** ▶ **Invited** 17:00–17:20**Molecular Recognition of Water Isotopes on Porous
Coordination Polymer**Hideki TANAKA¹, Shotaro HIRAIDE², Kazuhiro NAGAI²,
Abhishek BAGUSETTY³, J. Karl JOHNSON³,
Minoru T. MIYAHARA², Katsumi KANEKO¹, Katsuya TESHIMA¹
¹Shinshu University, ²Kyoto University, ³University of
Pittsburgh**H1-12-I20** ▶ **Invited** 17:20–17:40**Synthesis of Activated carbon with iron for water
treatment**Yuki KAMIMOTO
Nagoya University**H1-12-I21** ▶ **Invited** 17:40–18:00**Boron-Doped Diamond Powder as a Functional
Electrode Material**Takeshi KONDO
Tokyo University of Science**H1-12-I22** ▶ **Invited** 18:00–18:20**Separation and Purification Using Microporous
Materials**Takeshi HAGIO^{1,2}, Supinya NIJPANICH², Hiroto KUNISHI²,
Takaaki SAKASHITA², Yuki KAMIMOTO¹, Ryoichi ICHINO^{1,2,3}
¹Institute of Materials Innovation, Institutes of Innovation
for Future Society, Nagoya University, ²Department of
Chemical Systems Engineering, Graduate School of
Engineering, Nagoya University, ³Green Mobility Research
Institute, Institutes of Innovation for Future Society, Nagoya
University**H1-12-I23** ▶ **Invited** 18:20–18:40**Selective Removal of Nitrate ions by F-Substituted
Layered Double Hydroxides (LDHs): Purification of
Waste Water**Tomohito SUDARE¹, Masahiro KIYAMA², Fumitaka HAYASHI²,
Katsuya TESHIMA^{1,2}¹Research Initiative for Supra-Materials, Shinshu
University, ²Department of Materials Chemistry, Faculty of
Engineering, Shinshu University

December 11, 2019

Poster Session**Time** 11:30–13:00 **Room** Trade-0**H1-11-P01** ▶ **Invited****Anti-algae Effect of Water Treated by In-liquid Plasma
Bubbled with Air**Chiaki TERASHIMA
Tokyo University of Science**H1-11-P02****Advantages of Stimuli-responsive Amphiphiles for
Removal of Noble-metal Nanoparticles from Water**Clara IMURA, Yuko ANDA, Saki IJIMA
Ochanomizu University**H1-11-P03****Development of solution plasma technology for
sustainable nitrogen circulation system**Genji OKADA^{1,2,3}, Norihiro SUZUKI^{2,3}, Ken-ichi KATSUMATA^{2,3},
Yoshimi NISHIMURA⁴, Takeshi KONDO^{1,2}, Makoto YUASA^{1,2,3},
Akira FUJISHIMA², Chiaki TERASHIMA^{2,3,5}¹Tokyo University of Science, ²Photocatalysis International
Research Center, TUS, ³Research Center for Space Colony,
TUS, ⁴Kurita Manufacturing Co.,Ltd, ⁵Research Initiative for
Supra-Materials, Shinshu University**H1-11-P04****Pharmaceuticals Decomposition by Solution Plasma for
Application to Water Purification Technology**Yuki HIRAMI^{1,2,3}, Vicente Rodriguez GONZALEZ^{2,4},
Norihiro SUZUKI^{2,3}, Ken-ichi KATSUMATA^{2,3},
Takeshi KONDO^{1,2}, Yoshimi NISHIMURA⁵, Makoto YUASA^{1,2,3},
Akira FUJISHIMA², Chiaki TERASHIMA^{2,3,6}¹Graduation School of Science and Technology, Tokyo
University of Science, ²Photocatalysis International
Research Center, ³Research Center for Space Colony,
⁴Institute for Science and Technological Research of Sun
Luis Potosi, ⁵Kurita Manufacturing Co. Ltd., ⁶Research
Initiative for Supra-Materials**H1-11-P05****Evaluation of Formic Acid Adsorption Performance at
the Surface of Hydro-garnet Materials by First Principles
Calculation**Kunihiro ISHIDA¹, Kentarou WATANABE¹, Naoto TANIBATA^{1,2},
Masanobu NAKAYAMA^{1,2,3}, Hirotaka MAEDA¹¹Nagoya Institute of Technology, ²Kyoto University ESICB
of Elements Strategy Initiative for Catalysts and Batteries,
³MaDiS/CMi2, NIMS of National Institute for Materials
Science

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

H1-11-P06
Production of Liquid Fertilizer by Flow-type In-liquid Plasma Device

Mao SASAKI¹, Shoki SUZUKI^{1,2,3}, Norihiro SUZUKI^{2,3}, Ken-ichi KATSUMATA^{2,3}, Yoshimi NISHIMURA⁴, Takeshi KONDO^{1,2}, Makoto YUASA^{1,2,3}, Akira FUJISHIMA², Chiaki TERASHIMA^{2,3,5}

¹Tokyo University of Science, ²Photocatalysis International Research Center, ³Research Center for Space Colony, ⁴Kurita Manufacturing Co.,Ltd., ⁵Research Initiative for Supra-Materials

H1-11-P07
Spectroscopic Study for Fluorescein Adsorbed on TiO₂ Surface by Surface-Enhanced Infrared Absorption Spectroscopy

Hayato KONDO¹, Yosuke KAGESHIMA^{1,2}, Katsuya TESHIMA^{1,2}, Hiromasa NISHIKIORI^{1,2}

¹Department of Materials Chemistry, Faculty of Engineering, Shinshu University, ²Research Initiative for Supra-Materials (RISM), Shinshu University

H1-11-P08
Effective Utilization of Cellulose Thin Film Deposited on Porous TiO₂ Photoanode in a Photofuel Cell

Takumi YOSHIMURA¹, Yosuke KAGESHIMA^{1,2}, Katsuya TESHIMA^{1,2}, Hiromasa NISHIKIORI^{1,2}

¹Department of Materials Chemistry, Faculty of Engineering, Shinshu University, ²Research Initiative for Supra-Materials (RISM), Shinshu University

H1-11-P09
Advanced oxidation process for water purification using deep-ultraviolet light TiO₂ nano composite electrode

Akihiro OKAZAKI¹, Haruo KURIYAMA¹, Izumi SERIZAWA¹, Aiga HARA², Yui HIRANO², Yukihiko NAKABAYASHI², Nitish ROY², Norihiro SUZUKI², Chiaki TERASHIMA², Kazuya NAKATA², Ken-ichi KATSUMATA², Akira FUJISHIMA²

¹ORC Manufacturing, ²Tokyo University of Science

H1-11-P10
Formation of a silane/Mg(OH)₂ corrosion resistant composite film on flame-resistant AX41 alloy by combination of steam coating and spin coating treatments

Tomohiro MIYASHITA¹, Momo INAMURA¹, Hiraku MUTO¹, Takahiro ISHIZAKI²

¹Materials Science and Engineering, Graduate School of Engineering and Science, Shibaura Institute of Technology, ²Department of Materials Science and Engineering, College of Engineering, Shibaura Institute of Technology

H1-11-P11
Corrosion resistance of films formed on thermally treated Mg-6Al-1Zn-2Ca alloy by steam coating

Momo INAMURA¹, Tomohiro MIYASHITA¹, Hiraku MUTO¹, Takahiro ISHIZAKI²

¹Materials Science and Engineering, Graduate School of Engineering and Science, Shibaura Institute of Technology, ²Department of Materials Science and Engineering, College of Engineering, Shibaura Institute of Technology

H1-11-P12
Fabrication of Structural Controlled Carbon Nanotube Ultralight Material

Kazuki MATSUSHIMA, Naoto SHIOURA, Tomonaga UENO
Nagoya University

H1-11-P13
Effects of Particle Size of (ZnSe)_{0.85}(CuIn_{0.7}Ga_{0.3}Se₂)_{0.15} on Photoelectrochemical Performances in Sunlight-Driven Water Reduction

Fumiaki TAKAGI¹, Yosuke KAGESHIMA^{1,2}, Katsuya TESHIMA^{1,2}, Kazunari DOMEN^{1,2}, Hiromasa NISHIKIORI^{1,2}

¹Faculty of Engineering, Shinshu University, ²Research Initiative for Supra-Materials (RISM), Shinshu University

H1-11-P14
Corrosion resistance of composite hydroxides film formed on Al-Zn-Mg alloy by steam coating

Hiraku MUTO¹, Tomohiro MIYASHITA¹, Momo INAMURA¹, Takahiro ISHIZAKI²

¹Materials Science and Engineering, Graduate School of Engineering and Science, Shibaura Institute of Technology, ²Department of Materials Science and Engineering, Faculty of Engineering, Shibaura Institute of Technology

H1-11-P15
Generation of Hydrophobic Effect on Nickel 3D Structure by Electroplating

Shinya TAKO¹, Tomofumi MOCHIZUKI², Masahiro NAKAYAMA³, Yohei KOTSUCHIBASHI⁴, Katsuhiko TASHIRO^{5,6}, Hideo HONMA^{5,6}, Osamu TAKAI^{5,6}

¹Kanto Gakuin University Graduate School of Engineering, ²Hamamatsu Industrial Research Institute, ³Nakayama Precious Metal Plating Co. Ltd., ⁴Shizuoka Institute of Science and Technology, Department of Materials and Life Science, ⁵Kanto Gakuin University Materials and Surface Engineering Research Institute, ⁶Research Advancement and Management Organization, Kanto Gakuin University

H1-11-P16
One-pot Synthesis of MnO₂-Carbon Hybrids For Enhancement of the Cationic Dyes Removal

Hymin KIM¹, Seulgee LEE^{2,3}, Nagahiro SAITO^{2,4,5,6}

¹LG chem., ²Department Chemical Systems Engineering, Graduate School of Engineering, Nagoya University, ³Division of Marine Engineering, Korea Maritime and Ocean University, ⁴Conjoint Research Laboratory in Nagoya University, Shinshu University, ⁵Japan Science and Technology Corporation (JST), Open Innovation Platform with Enterprises, Research Institute and Academia (OPERA), ⁶Japan Science and Technology Corporation (JST), Strategic International Collaborative Research Program (SICORP)

H1-11-P17
Molecular orientation control in a PEDOT transparent conductive film by hydrodynamic interaction

Yushi FUJITA¹, Keita YASUMORO¹, Takuya FUJIMA^{1,2}

¹Department of Mechanical Engineering / Tokyo City University, ²Advanced Research Laboratories, Tokyo City University

H1-11-P18**Flux Growth of Layered Sodium Titanate Crystals with Hierarchical Structure for Water Purifier Application**

Taichi SAKAMAKI¹, Fumitaka HAYASHI¹,
Tomohito SUDARE², Katsuya TESHIMA^{1,2}

¹Department of Materials Chemistry, Shinshu University,
²Research Initiative for Supra-Materials, Shinshu University

H1-11-P19**Highly-stable Glucose/Oxygen Biofuel Cell based on Carbon Cloth Electrodes modified with Poly(glycidyl methacrylate)-grafted MgO-templated Porous Carbon**

Takanao KATO¹, Yoshinao HOSHI¹, Isao SHITANDA^{1,2},
Masayuki ITAGAKI^{1,2}, Seiya TSUJIMURA^{2,3}

¹Department of Pure and Applied Chemistry, Faculty of
Science and Technology, Tokyo University of Science,
²Research Institute for Science and Technology, Tokyo
University of Science, ³Division of Material Science, Faculty
of Pure and Applied Science

H1-11-P20**Durability of Hierarchical Nanoporous Layer Glass Functionality at High Temperature**

Takumi ITO¹, Erika TABATA¹, Yuki USHIODA¹,
Takuya FUJIMA^{1,2}

¹Department of Mechanical Engineering, Tokyo City
University, ²Advanced Research Laboratories, Tokyo City
University

H1-11-P21**Flux Growth of Single-Crystalline, Layered K₂Ti₂O₅ Particles and Their Ion Exchange Property**

Nanako TATEWAKI¹, Fumitaka HAYASHI¹,
Tomohito SUDARE², Katsuya TESHIMA^{1,2}

¹Department of Materials Chemistry, Shinshu University,
²Research Initiative for Super-Materials, Shinshu University

H1-11-P22**Gas-Liquid Interfacial Plasma Polymerization of EDOT**

Jun-Seok OH, Shunta HIRANO, Ryoga KONISHI,
Tatsuru SHIRAFUJI
Osaka City University

H1-11-P23**Renovation Water Permeability of a Continuous Porous Dielectric Using Propagation of Plasma Bullets**

Tatsuru SHIRAFUJI, Yuki HAMAMOTO, Ryo MATOBA,
Jun-seok OH
Osaka City University

H1-11-P24**Screen-printing of Chitosan Film for Improvement of Paper-based Lactate Biofuel Cell Stability**

Kanako ODA¹, Yoshinao HOSHI¹, Isao SHITANDA^{1,2},
Masayuki ITAGAKI^{1,2}, Seiya TSUJIMURA^{2,3},
Abdelkader ZEBDA⁴

¹Department of Pure and Applied Chemistry, Faculty of
Science and Technology, Tokyo University of Science,
²Research Institute for Science and Technology, Tokyo
University of Science, ³Division of Material Science, Faculty
of Pure and Applied Science, University of Tsukuba, ⁴UGA-
Grenoble 1/CNRS/INSERM/TIMC-IMAG UMR 5525

H1-11-P25**Development of a highly durable PEDOT transparent conductive film using a macro-separated composition**

Keita YASUMURO¹, Yushi FUJITA¹, Takuya FUJIMA^{1,2}

¹Department of Mechanical Engineering, Tokyo City University,
²Advanced Research Laboratories, Tokyo City University

December 11, 2019

Poster Session

Time 19:00–20:30	Room Trade-0
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H1-11-P26 ▶ Invited**Flux Crystal Growth Innovation for Advanced Water Science and Technology**

Katsuya TESHIMA
Shinshu University

H1-11-P27**Synthesis of Phosphorus-doped Diamond by In-liquid Microwave Plasma CVD Process**

Akihiro UCHIDA¹, Chiaki TERASHIMA^{1,2}, Hiroshi UETSUKA^{1,3},
Norihiro SUZUKI¹, Ken-ichi KATSUMATA¹, Masayuki ITAGAKI¹,
Isao SHITANDA¹, Yoshinao HOSHI¹, Takeshi KONDO¹,
Akira FUJISHIMA¹

¹Tokyo University of Science, ²Shinshu University, ³Asahi
Diamond Industrial Co., Ltd.

H1-11-P28**Development of photocatalytic HTiO_{2-x} by plasma treatment in liquid**

Junki ISHII^{1,2}, Shoki SUZUKI^{1,2}, Norihiro SUZUKI²,
Ken-ichi KATSUMATA², Kazuya NAKATA^{1,2}, Takeshi KONDO^{1,2},
Makoto YUASA^{1,2}, Akira FUJISHIMA², Chiaki TERASHIMA²

¹Tokyo University of Science, ²Photocatalysis International
Research Center

H1-11-P29**Protection of the important cultural property using a self-cleaning effect by the photocatalyst**

Kazuki KATO^{1,2}, Chiaki TERASHIMA², Norihiro SUZUKI²,
Ken-ichi KATSUMATA², Takeshi KONDO^{1,2}, Makoto YUASA^{1,2},
Akira FUJISHIMA², Tomonori SUZUKI³

¹Department of Pure and Applied Chemistry, Tokyo
University of Science, ²Photocatalysis International
Research Center, Tokyo University of Science, ³Department
of Applied Biological Science, Tokyo University of Science

H1-11-P30

Development of Selective Hydrophilic / Hydrophobic Surface Treatment for Semiconductor Substrate

 Hiroshi IKARI¹, Chiaki TERASHIMA², Norihiro SUZUKI², Ken-ichi KATSUMATA², Takeshi KONDO^{1,2}, Makoto YUASA^{1,2}, Akira FUJISHIMA²
¹Graduate School of Science and Technology, Tokyo University of Science, ²Photocatalysis International Research Center

H1-11-P31

Fabrication of Ni-Co Layered Double Hydroxides via Topotactic Reaction for Efficient Removal of Nitrate Ions : Purification of Waste Water

 Shuhei TAMURA¹, Tomohito SUDARE², Fumitaka HAYASHI¹, Katsuya TESHIMA^{1,2}
¹Department of Materials Chemistry, Shinshu University, ²Research Initiative for Supra-Materials, Shinshu University

H1-11-P32

Concentration of trace components in the environmental water using freezing and melting process of eutectics of salt and water

 Yuko NISHIMOTO, Masaru ARAI
Kanagawa Univ.

H1-11-P33

Analysis on Biocathode based on MgO-templated Carbon-modified Carbon Cloth by 3D Impedance Spectroscopy

 Hiromichi INOUE¹, Yoshinao HOSHI¹, Isao SHITANDA^{1,2}, Masayuki ITAGAKI^{1,2}, Seiya TSUJIMURA^{2,3}
¹: Department of Pure and Applied Chemistry, Faculty of Science and Technology, Tokyo University of Science, ²Research Institute for Science and Technology, Tokyo University of Science, ³Division of Material Science, Faculty of Pure and Applied Science, University of Tsukuba

H1-11-P34

Liquid Phase Plasma Synthesis of Amino-Rich Carbonaceous as an Efficient Adsorbent for Removal of Heavy Metal Ions

 Mongkol TIPPLOOK¹, Andres Eduardo ROMERO VALENZUELA¹, Nagahiro SAITO^{1,2,3,4}
¹Department of Chemical System Engineering, Graduate School of Engineering, Nagoya University, ²Conjoint Research Laboratory in Nagoya University, Shinshu University, ³Japan Science and Technology Corporation (JST), Open Innovation Platform with Enterprises, Research Institute and Academia (OPERA), ⁴Japan Science and Technology Corporation (JST), Strategic International Collaborative Research Program (SICORP)

H1-11-P35

Fabrication of Porous Silica / Carbon Nanotube Composite Materials for Thermal Insulator

 Naoto SHIOURA¹, Kazuki MATSUSHIMA¹, Tomoki OSATO¹, Tomonaga UENO¹, Norifumi ISU², Takeshi HASHIMOTO³, Takumi YANA³
¹Nagoya University, ²LIXIL Corp., ³Meijo Nano Carbon Co., Ltd.

H1-11-P36 ▶ Invited

Pattern formation in heterostructured medium by reaction-diffusion system

 Tomonaga UENO
Nagoya University

H1-11-P37

Capillary Condensation on Hierarchical Nanoporus Layer Glass

 Erika TABATA¹, Yuki USHIODA¹, Takumi ITO¹, Takuya FUJIMA^{1,2}
¹Faculty of Engineering, Tokyo City University, ²Advanced Research Laboratories, Tokyo City University

H1-11-P38

Surface modification of B-doped diamond using H₂O RF plasma

 Yukihiro SAKAMOTO
Chiba Institute of Technology

H1-11-P39

A Porous Layer Formation on Glaze for a Superhydrophilic Anti-Fouling Tile

 Yuki USHIODA¹, Erika TABATA¹, Takumi ITO¹
¹Department of Mechanical Engineering Tokyo City University, ²Advanced Research Laboratories Tokyo City University

H1-11-P40

Study on Aging Effect of Adhesion Strength between Polyimide Film and Copper Layer

 Changmyeon LEE^{1,2}, Hongkee LEE², Hideo HONMA^{1,3}, Osamu TAKAI³, Joo-Hyong NOH^{1,3}, Jun-Mi JEON²
¹Graduate School of Engineering/Kanto Gakuin University, ²Surface treatment group/Korea Institute of Industrial Technology, ³Materials and Surface Engineering Research Institute/Kanto Gakuin University

H1-11-P41 ▶ Invited

Protein adsorption behavior on reduced graphene oxide and boron-doped diamond

 Madoka TAKAI¹, Chiaki TERASHIMA², Yixuan HUANG¹
¹The University of Tokyo, ²Tokyo University of Science

H1-11-P42

Flash Lamp Annealing Effect on low-dielectric thin film

 Byeong-Jae CHOI^{1,2}, Jong-Young PARK^{1,2,3}, Hideo HONMA^{1,2}, Joo-Hyong NOH^{1,2}
¹Graduate School of Engineering, Kanto Gakuin University, ²Materials and Surface Engineering Research Institute, Kanto Gakuin University, ³Daeduck Electronics Co. Ltd.

H1-11-P43

Flux Growth of Crystalline Titanosilicate K₂TiSi₃O₉ Hexagonal Plates for Water Purifier Application

 Fumitaka HAYASHI¹, Mizuho KIYOHARA¹, Yongsu KIM¹, Tomohito SUDARE², Katsuya TESHIMA^{1,2}
¹Department of Materials Chemistry, Shinshu University, ²Research Initiative for Supra-Materials, Shinshu University

H1-11-P44**Ion Exchange Properties of NiFe Layered Double Hydroxides Crystals Fabricated via Topotactic Reaction: Purification of Waste Water**

Kazuki HIRONO¹, Tomohito SUDARE², Fumitaka HAYASHI¹, Katsuya TESHIMA^{1,2}

¹Department of Materials Chemistry, Shinshu University,

²Research Initiative for Supra-Materials, Shinshu University

H1-11-P45**Painted Diamond Electrode for Electrolytic Water Treatment**

Takeshi KONDO¹, Haruka NAKAJIMA¹, Shuji EZURA¹, Eiichi KANEDA², Toshifumi TOJO¹, Makoto YUASA¹

¹Tokyo University of Science, ²A1 Technica Co., Ltd.

H1-11-P46**Sensitive Detection of Ciprofloxacin at Screen-Printed Diamond Electrode by Control of Surface Termination of Boron-Doped Diamond Powder**

Tomohiro MATSUNAGA, Takeshi KONDO, Toshifumi TOJO, Makoto YUASA

Tokyo University of Science

H1-11-P47**Application of Boron-Doped Nanodiamond to Aqueous Supercapacitors**

Seiya SUGAI¹, Kenjo MIYASHITA¹, Takeshi KONDO¹, Masahiro NISHIKAWA², Takehiro TEI², Toshifumi TOJO¹, Makoto YUASA¹

¹Tokyo University of Science, ²Daicel Corporation

H1-11-P48**Evaluation of Wettability and Corrosion Resistance of SiO:CH Coatings Deposited on SUS304 Substrate by PECVD**

Mamoru YAZAKI¹, Masahiro KANNO¹, Kyosuke KUREHA¹, Yasushi INOUE¹, Osamu TAKAI²

¹Chiba Institute of Technology, ²Kanto Gakuin University

H1-11-P49**Analysis of Local Ion Concentration Near Membrane by Dynamic Complex Impedance Measurement in Electrolyte / Reverse Osmosis Membrane System**

Atsushi TANAKA^{1,2}, Hirosuke TATSUMI³, Katsuya TESHIMA^{1,2}

¹Research Initiative for Supra-Materials, Shinshu University,

²Global Aqua innovation Center, Shinshu University,

³Department of Science, Shinshu University

H1-11-P50**Study of Bacterial Adhesion Strength on Phospholipid Copolymer Coating Surfaces by Analysis with Microchannel**

Madoka TAKAI¹, Zhou LU¹, Tsukuru MASUDA¹, Norifumi ISU²

¹The University of Tokyo, ²LIXIL corporation

December 11–13, 2019

Symposium H-2

Plasma-Based Synthesis, Processing and Characterization of Materials for Energy and Environment

[Organizers]

Masaharu SHIRATANI (Kyushu University)
 Kunihiko KAMATAKI (Kyushu University)
 Kazuo TERASHIMA (The University of Tokyo)
 Yuichi SETSUHARA (Osaka University)
 Jin-Hyo BOO (Sungkyunkwan University)
 Uroš CVELBAR (Jožef Stefan Institute)

December 11, 2019

Oral Session 1

Time 9:00–11:30 **Room** Mont-3

Chairperson Hajime SHIRAI

H2-11-I01 ▶ Invited 9:00–9:30

Low Temperature Plasma Deposition Processes: From Amorphous Silicon to Epitaxial Growth and Nanowires

Pere ROCA I CABARROCAS

LPICM, CNRS, Ecole polytechnique

H2-11-002 9:30–9:45

Defect Control of Plasma Synthesized Free-standing Silicon Nanocrystals

Shogo SHIBATA, Shuhei WAKAMATSU,
Firman Bagja JUANGSA, Tomohiro NOZAKI

Tokyo Institute of Technology

H2-11-003 9:45–10:00

Printable Organic-Inorganic Hybrid Solar Cell via Silicon Inks

Munehika OTSUKA¹, Yi DING², Shogo SHIBATA¹,
Firman Bagja JUANGSA¹, Yuki KUROKAWA³,
Takehito KATO³, Tomohiro NOZAKI¹

¹Department of Mechanical Engineering, Tokyo Institute of Technology, ²Institute of Photoelectronic Thin Film Devices and Technology, Nankai University, ³Department of Mechanical Engineering, National Institute of Technology, Oyama College

H2-11-I04 ▶ Invited 10:00–10:30

Highly transparent Pt-free dye-sensitized solar cells

Hyunwoong SEO

Department of Energy Engineering, Inje University

H2-11-005 10:30–10:45

Therma- and plasma-ALD Al₂O₃/n-Si field effect inversion layer for PEDOT:PSS/n-Si heterojunction solar cells

Md Enamul KARIM¹, Arifuzzaman RAJIB¹, Tomofumi UKAI²,
A.T.M. Saiful ISLAM¹, Shunji KUROSU², Yasuhiko FUJII²,
Masahide TOKUDA², Tatsuro HANAJIRI², Ryo ISHIKAWA¹,
Keiji UENO¹, Hajime SHIRAI¹

¹Saitama University, ²Toyo University

H2-11-I06 ▶ Invited 10:45–11:15

Plasma Process Silicon Quantum Dots and Perovskites Hybrids for PV

Vladimir SVRCEK¹, Calum MCDONALD¹, Conor ROCKS^{1,2},
Davide MARIOTTI², Takuya MATSUI¹

¹AIST Tsukuba, ²University of Ulster, BT37 0QB, Northern Ireland, UK

H2-11-007 11:15–11:30

Highly-transparent photovoltaic cell based on atomically thin 2D materials

Xing HE¹, Yoshiki YAMAGUCHI¹, Toshiro KANEKO¹,
Toshiaki KATO^{1,2}

¹Tohoku University, ²JST-PRESTO

December 11, 2019

Oral Session 3

Time 16:30–18:30 **Room** Mont-3

Chairperson Kunihiko KAMATAKI

H2-11-I08 ▶ Invited 16:30–17:00

Photoelectrochemical Water Splitting for Hydrogen Production with Ternary Oxide Materials

Min-Kyu SON

Kyushu University

H2-11-009 17:00–17:15

Kinetic study of plasma mediated heterogeneous catalysis of biogas

Yoshiki WATANABE, Kenta SAKATA, Seigo KAMESHIMA,
Zunrong SHENG, Tomohiro NOZAKI

Tokyo Institute of Technology

H2-11-010 17:15–17:30

Non-thermal plasma as a powerful tool to synthesize bio-effective materials in solutions

Hiromasa TANAKA, Masaaki MIZUNO, Kenji ISHIKAWA,
Hiroki KONDO, Hiroshi HASHIZUME, Yasumasa OKAZAKI,
Shinya TOYOKUNI, Kae NAKAMURA, Nobuhisa YOSHIKAWA,
Hiroaki KAJIYAMA, Fumitaka KIKKAWA, Masaru HORI

Nagoya University

H2-11-I11 ▶ Invited 17:30–18:00

Plasmon-Enhanced Plasma Processing of N-doped Graphene for Fuel-cell Catalysts

Takeshi KITAJIMA, Ginga SATOH, Toshiki NAKANO

National Defense Academy

H2-11-I12 ▶ Invited 18:00–18:30

Investigation of Impact of Plasma Fluctuation Driven by Amplitude Modulated VHF Discharge on Growth of Nanoparticles in Reactive Plasma

Kunihiro KAMATAKI, Ryosuke IWAMOTO, Hayate TANAKA, Daisuke YAMASHITA, Naho ITAGAKI, Kazunori KOGA, Masaharu SHIRATANI
Kyushu University

December 12, 2019

Oral Session 4

Time 9:00–11:30 Room Work-3

Chairperson Hiroki KONDO

H2-12-I01 ▶ Invited 9:00–9:30

Facile improvement in cycle capacity with PFE Si:SnOx nanocomposites for lithium secondary batteries

Makoto KAMBARA
The University of Tokyo

H2-12-I02 ▶ Invited 9:30–10:00

High-Speed Visualization of Metal Oxide Precursor in Thermal Plasma during Nanoparticle Synthesis Process

Manabu TANAKA, Yuki SAITO, Takayuki WATANABE
Kyushu University

H2-12-003 10:00–10:15

Formation Mechanism of Tungsten Boride Nanoparticles by Induction Thermal Plasma

Libei LIU, Yuta TANQUE, Manabu TANAKA, Takayuki WATANABE
Kyushu University

Break
10:15–10:30

H2-12-004 10:30–10:45

Reaction Mechanisms of High-Fluorine-Content Reactive Ion etching (RIE) and Atomic Layer Etching (ALE) of Si and SiO₂

Erin Joy Capdos TINACBA
Osaka University

H2-12-005 10:45–11:00

Energy distribution measurement of substrate incident charged particles in DC magnetron discharge of oxide target

Masaki ISHIBA
Graduate School of Engineering, Nagasaki University

H2-12-I06 ▶ Invited 11:00–11:30

Development of a direct bonding process by using high-frequency Ar plasma jet

Giichiro UCHIDA¹, Rikuro MACHIDA², Kosuke TAKENAKA², Yuichi SETSUHARA²
¹Meijo University, ²Osaka University

December 12, 2019

Oral Session 6

Time 16:30–18:30 Room Work-3

Chairperson Takeshi KITAJIMA

H2-12-I07 ▶ Invited 16:30–17:00

Synthesis of Carbon Nanostructures using Microwave-Exited Atmospheric Pressure Plasma

Mineo HIRAMATSU¹, Koki MIYASHITA¹, Taishu OYAMA¹, Keigo TAKEDA¹, Hiroki KONDO², Masaru HORI²
¹Meijo University, ²Nagoya University

H2-12-008 17:00–17:15

Apparent Activation Energy of Sabatier Reaction in Low Pressure Plasma-Catalyst Gas Conversion

Masaharu SHIRATANI
Kyushu University

H2-12-009 17:15–17:30

Atomic hydrogen exposures of radical-injection CH₄/H₂ plasma-enhanced chemical vapor deposited amorphous carbon films

Yasuyuki OHASHI, Hiroki KONDO, Kenji ISHIKAWA, Takayoshi TSUTSUMI, Makoto SEKINE, Masaru HORI
University of Nagoya

H2-12-010 17:30–17:45

Utilization of microwave-induced plasma in extremely fast activation for preparation of activated carbon with large surface area

Purichaya KUPTAJIT, Noriaki SANO
Kyoto University

H2-12-011 17:45–18:00

Fabrication of graphene nanoribbon-based quantum device with plasma CVD

Mizuki SEO¹, Wakana OKITA¹, Hiroo SUZUKI¹, Toshiro KANEKO¹, Toshiaki KATO^{1,2}
¹Tohoku University, ²JST-PRESTO

H2-12-012 18:00–18:15

Chirality selective growth of (6,4) single-walled carbon nanotubes by plasma CVD

Satoru SHIINA¹, Takuya SHIMA¹, Bin XU¹, Toshiro KANEKO¹, Toshiaki KATO^{1,2}
¹Tohoku University, ²JST-PRESTO

H2-12-013 18:15–18:30

Synthesis and crystallinity of nanographene using in-liquid plasma of ethanol

Ryo HAMAJI¹, Hiroki KONDO¹, Takayoshi TSUTSUMI¹, Kenji ISHIKAWA¹, Makoto SEKINE¹, Keigo TAKEDA², Mineo HIRAMATSU², Masaru HORI¹
¹University of Nagoya, ²University of Meijo

December 13, 2019

Oral Session 7
Time 9:00–11:30 **Room** Work-3

 Chairperson Giichiro UCHIDA
H2-13-001 9:00–9:15

Decomposition of vanillin and lignin using pulsed low current arc in ambient air for production of biocellulosic ethanol

Vladislav GAMALEEV¹, Naoyuki IWATA¹, Ginji ITO¹, Motoyuki SHIMIZU², Masashi KATO², Mineo HIRAMATSU¹, Masafumi ITO¹
¹Faculty of Science and Technology, Meijo University,

²Faculty of Agriculture, Meijo University

H2-13-002 9:15–9:30

 Modification of lipid metabolism in *Coccomyxa* sp. treated by non-equilibrium atmosphere pressure plasma

Takumi KATO
 Nagoya University

H2-13-003 9:30–9:45

 Role Of Water For The Mist-CVD Of Al₂O₃
Arifuzzaman RAJIB¹, Md Enamul KARIM¹, Koki IMAI¹, Tomofumi UKAI², Shunji KUROSU², Yasuhiko FUJII², Masahide TOKUDA², Tatsuro HANAJIRI², Ryo ISHIKAWA¹, Keiji UENO¹, Hajime SHIRAI¹
¹Saitama University, ²Toyo University

H2-13-004 9:45–10:00

Growth Promotion Effect of Oxygen-Radical-Treated Phenylalanine Solutions

Naoyuki IWATA¹, Vladislav GAMALEEVE¹, Hiroshi HASHIZUME², Jun-Seok OH³, Takayuki OHTA¹, Kenji ISHIKAWA², Masaru HORI², Masafumi ITO¹
¹Meijo University, ²Nagoya University, ³Osaka City University

H2-13-I05 ▶ Invited 10:00–10:30

 Changes of resistive elements during degradation of carbon nanowalls electrodes for fuel cell synthesized employing a CH₄/H₂ mixture gas plasma

Hiroki KONDO¹, Shun IMAI¹, Takayoshi TSUTSUMI¹, Kenji ISHIKAWA¹, Makoto SEKINE¹, Mineo HIRAMATSU², Masaru HORI¹
¹Nagoya University, ²Meijo University

H2-13-006 10:30–10:45

 Fabrication of SiNx films using SiH₄+N₂ multi hollow discharge plasma CVD method: Effects of total gas flow rate

Yusuke SASAKI
 Kyushu University

H2-13-I07 ▶ Invited 10:45–11:15

Sputtering Deposition with Impurities: Another Key Parameter to Control Film Structures

Naho ITAGAKI, Kunihiro KAMATAKI, Kazunori KOGA, Masaharu SHIRATANI
 Kyushu University

Closing Remarks

11:15–11:30

December 12, 2019

Poster Session
Time 14:00–15:30 **Room** Trade-0

H2-12-P01

Two-dimensional functional thin film preparation by sputtering deposition using powder targets

Hiroharu KAWASAKI
 National Institute of Technology, Sasebo College

H2-12-P02

Thin film preparation for preventing hydrogen embrittlement using sputtering deposition method

Hiroharu KAWASAKI
 National Institute of Technology, Sasebo College

H2-12-P03

Influence of Solute Atom Radius on Adsorption-induced Electrochromic Phenomenon of InN Films

Masahiro HOMMA^{1,2,3}, Yasushi INOUE¹, Osamu TAKAI⁴
¹Chiba Institute of Technology, ²The Japan Society of Applied Physics, ³Materials Science Society of Japan, ⁴Kantou Gakuin Univ

H2-12-P04

Preparation of Transparent Conductive Oxide Thin Film Using Mixed Powder Target by Sputtering Method: Control of Mixing Ratio

Tamiko OHSHIMA¹, Masaki NAKAMURA¹, Hiroharu KAWASAKI¹, Masanori SHINOHARA¹, Yoshihito YAGYU¹, Takeshi IHARA¹, Yoshiaki SUDA²
¹National Institute of Technology, Sasebo College, ²National Institute of Technology, Ishikawa College

H2-12-P05

Plasma-assisted Reactive Process for Fabrication of High Mobility IGZO Thin Film Transistor at Low-Temperature

Kosuke TAKENAKA¹, Hiroyuki HIRAYAMA¹, Giichiro UCHIDA², Akinori EBE³, Yuichi SETSUHARA¹
¹Joining and Welding Research Institute, Osaka University, ²Faculty of Science and Technology, Meijo University, ³EMD Corporation

H2-12-P06**Plasma Surface Modification towards Application of Polymers to Biomaterials**

Kosuke TAKENAKA, Yuichi SETSUHARA
Osaka University

H2-12-P07**Influence of Substrate Morphology on Microstructure of InN Films Fabricated by Glancing-angle Reactive Sputtering**

Masashi HOSOYA¹, Yasushi INOUE¹, Osamu TAKAI²
¹Chiba Institute Of Technology, ²Kanto Gakuin University

H2-12-P08**Comparison of Deposited Layers Using Three Different Thermal Sprays**

Yasuyuki KAWAGUCHI
Kyushu University

H2-12-P09**Surface Modification of Molybdenum Disulfide Synthesized from Molybdenum Thin Film**

Akihisa OGINO, Masachika TSUZUKI
Shizuoka University

H2-12-P10**Electromechanically High Sensitive Dielectric Elastomer as Composite of Polyrotaxane/Solution Plasma Surface Modified Graphene Aligned with External Electric Field.**

Kaito NAGAYAMA¹, Taku GOTO^{1,2}, Koichi MAYUMI¹,
Kazuto HATAKEYAMA², Yoshiki SHIMIZU², Tsuyohito ITO¹,
Kohzo ITO¹, Yukiya HAKUTA², Kazuo TERASHIMA^{1,2}
¹The University of Tokyo, ²National Institute of Advanced Industrial Science and Technology

H2-12-P11**Preparation of Carbon Nanomaterials by Atmospheric Pressure Gliding Arc Discharge**

Shin-ichi AOQUI
Sojo University

H2-12-P12**Reduction of graphene oxide by gas-liquid interface plasma**

Takayuki OHTA¹, Ikumi OHSAWA¹, Takahiro SAIDA²
¹Department of Electrical and Electronic Engineering, Meijo University, ²Department of Applied Chemistry, Meijo University

H2-12-P13**Effects of Pulse Bias Voltage on Characteristics of a-C:H Film Deposited by High Pressure Ar+CH₄ Plasma CVD Process**

SungHwa HWANG¹, Ryosuke IWAMOTO¹,
Kunihiro KAMATAKI¹, Naho ITAGAKI¹, Kazunori KOGA^{1,2},
Masaharu SHIRATANI¹
¹Kyushu University, ²National Institutes of Natural Science

H2-12-P14**Effects of higher-order silane molecules on Si-H₂ bond and Si-H bond densities in a-Si:H films.**

Hisayuki HARA, Yuan HAO, Kohei ABE, Daisuke YAMASHITA,
Kunihiro KAMATAKI, Naho ITAGAKI, Kazunori KOGA,
Masaharu SHIRATANI
Kyushu University

H2-12-P15**Developing Prediction of Amorphization Condition Models from Sputter Deposition Experimental Results by Machine Learning Method**

Kunihiro KAMATAKI, Ryosuke IWAMOTO, Sakyō OKUNAGA,
Soichiro MURAOKA, Daisuke YAMASHITA, Naho ITAGAKI,
Kazunori KOGA, Masaharu SHIRATANI
Kyushu University

H2-12-P16**Plasma-assisted CO₂ methanization in cryogenic condition**

Hayato KASAGAWA
The University of Tokyo

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 11–13, 2019

Symposium H-3

5th E&J BLS

Advanced Functional Oxides: Processing, Characterization and Devices

[Organizers]

Tetsuya YAMAMOTO (Kochi University of Technology)
 Nobuyuki IWATA (Nihon University)
 Kohei FUJIWARA (Tohoku University)
 Valentin Craciun (National Institute for Laser, Plasma and Radiation
 Physics and Extreme Light Infrastructure-NP)
 Hiroaki NISHIKAWA (Kindai University)
 Tetsuo TSUCHIYA (National Institute of Advanced Industrial
 Science and Technology)
 Florencio Sanchez (Institut de Ciencia de Materials de Barcelona)
 Robert L. Z. Hoye (University of Cambridge)
 Shunichi ARISAWA (National Institute for Materials Science)

December 11, 2019

Oral Session 1

Time 9:00–11:20 Room Miel-2

 Chairpersons Tetsuya YAMAMOTO, Hiroshi KAGEYAMA,
 Tetsuo TSUCHIYA

Opening Talk

9:00–9:10

H3-11-K01 ▶ Keynote 9:10–10:10

New Frontiers in Oxides Science with Multiple Anions

 Hiroshi KAGEYAMA
 Kyoto University

Break

10:10–10:20

H3-11-002 10:20–10:35

Unique electronic structure of ZnO crystals with the retained Ar atoms

 Tetsuya YAMAMOTO¹, Hisao MAKINO¹, Junichi NOMOTO²,
 Tomohiko NAKAJIMA², Tetsuo TSUCHIYA²
¹Kochi University of Technology, ²National Institute of
 Advanced Industrial Science and Technology

H3-11-003 10:35–10:50

Characterization of planar ZnO microcavities for the near ultraviolet polariton laser operatable at room temperature

 Kohei SHIMA, Kentaro FURUSAWA, Kazunobu KOJIMA,
 Shigefusa F CHICHIBU
 Tohoku University

H3-11-004

10:50–11:05

Light-Stimulated Synaptic Functionality in Solution Processed Zinc-Tin Oxide (ZTO) Thin Film Transistor

 Jen-Sue CHEN¹, Ting-Ruei LIN¹, Po-Jen CHENG¹,
 Sheng-Rong LIN¹, Yen-Hsun SU¹, Jih-Jen WU²,
 Chao-Cheng KAUN³
¹National Cheng Kung University, Dept. Materials Science
 and Engineering, ²National Cheng Kung University, Dept.
 Chemical Engineering, ³Academia Sinica, Research Center
 for Applied Sciences

H3-11-005

11:05–11:20

Growth and characterization RS-ZnCdO thin films on MgO(100) substrates by molecular beam epitaxy

 Jang HYOCHANG¹, Katsuhiko SAITO¹, Qixin GUO¹,
 Tooru TANAKA¹, Man Yu KIM², Wladek WALUKIEWICZ^{3,4}
¹Saga University, ²City University of Hong Kong, ³Lawrence
 Berkeley National Laboratory, ⁴University of California at
 Berkeley

December 11, 2019

Oral Session 3

Time 16:30–18:30 Room Miel-2

Chairpersons Valentin CRACIUN, Florencio SANCHEZ

H3-11-I06 ▶ Invited

16:30–17:05

New Capabilities and Characterization Tools for Atmospheric Pressure Spatial Deposition of Oxide Thin films

 Kevin MUSSELMAN^{1,2}, Kissan MISTRY^{1,2}, Alexander JONES^{1,2},
 Abdullah ALSHEHRI^{1,2}, Jhi YONG LOKE¹
¹Dept. of Mechanical and Mechatronics Engineering,
 University of Waterloo, ²Waterloo Institute for
 Nanotechnology, University of Waterloo

H3-11-007

17:05–17:20

Carrier transport of ultrathin Sn-doped In₂O₃ films grown by reactive plasma deposition

 Yutaka FURUBAYASHI¹, Makoto MAEHARA²,
 Hisashi KITAMI^{1,2}, Toshiyuki SAKEMI², Hisao MAKINO¹,
 Tetsuya YAMAMOTO¹
¹Kochi University of Technology, ²Sumitomo Heavy
 Industries, Ltd.

H3-11-008

17:20–17:35

Manipulation of carrier density for Sn-doped In₂O₃ films by irradiation of negatively ionized oxygen ions

 Yutaka FURUBAYASHI¹, Makoto MAEHARA²,
 Hisashi KITAMI^{1,2}, Toshiyuki SAKEMI², Hisao MAKINO¹,
 Tetsuya YAMAMOTO¹
¹Kochi University of Technology, ²Sumitomo Heavy
 Industries, Ltd.

Break

17:35–17:45

H3-11-009 17:45–18:00

In₂O₃-based Thin Film Transistor Fabricated by Direct Nanoimprint TechniqueEisuke TOKUMITSU

Japan Advanced Institute of Science and Technology

H3-11-010 18:00–18:15

Comparative Studies of the Composition and Structure of Various Tungsten Oxide Thin FilmsValentin CRACIUN^{1,6}, Hisao MAKINO², Doina CRACIUN¹, Petronela GAROI¹, Maria Diana DRACEA³, Dan PANTELICA³, Nathan C. OU⁴, Lisa MCELWEE-WHITE⁴, Marian MOGILDEA⁵, George MOGILDEA⁵¹National Institute for Laser, Plasma and Radiation Physics,²Kochi University of Technology, ³Horia Hulubei NationalInstitute for Physics and Nuclear Engineering, ⁴Universityof Florida, ⁵Institute of Space Science, ⁶Extreme Light

Infrastructure for Nuclear Physics

H3-11-011 18:15–18:30

Optical properties and Rietveld refinement of Ca₃WO₆ : Eu³⁺ phosphorsTakahito OTSUKA, Tomokatsu HAYAKAWA

Nagoya Institute of Technology

December 12, 2019

Oral Session 4**Time** 9:00–11:25 **Room** Work-2Chairpersons Shunichi ARISAWA, Robert L.Z. HOYE

H3-12-101 ▶ Invited 9:00–9:35

Effect of air processing on the transport properties of ZnO:Al thin films. A new conductivity modelDavid MUÑOZ-ROJAS, Viet Huong NGUYEN, Daniel BELLET

Laboratoire des Matériaux et du Génie Physique (CNRS - Grenoble INP)

H3-12-002 9:35–9:50

Manipulation of growth and oxygen-related point defects of Ga-doped ZnO polycrystalline films by controlling direct-current arc plasmaHisashi KITAMI^{1,3}, Junichi NOMOTO², Toshiyuki SAKEMI¹, Yutaka FURUBAYASHI³, Hisao MAKINO³, Tetsuya YAMAMOTO³¹Sumitomo Heavy Industries, Ltd., ²National Institute of Advanced Industrial Science and Technology (AIST), ³Kochi University of Technology

H3-12-003 9:50–10:05

Sequential Compensation Effect of Anion/Cation Vacancies on Thermal Stability of Electrical Conductivity of Al-doped ZnO NanofilmsRuolin YAN, Tsunaki TAKAHASHI, Masaki KANAI, Takuro HOSOMI, Guozhu ZHANG, Kazuki NAGASHIMA, Takeshi YANAGIDA

Kyushu University

Break
10:05–10:15

H3-12-104 ▶ Invited 10:15–10:50

Upconversion phosphors for optical thermometer and solar cellsHendrik C SWART, Ashwini KUMAR, RE KROON, JJ TERBLANS, Govind B NAIR

University of the Free State

H3-12-105 ▶ Invited 10:50–11:25

Novel materials for stable perovskite solar cellsAntonio ABATE

Helmholtz-Zentrum Berlin

December 12, 2019

Oral Session 6**Time** 16:30–18:30 **Room** Work-2Chairpersons Kohei FUJIWARA, Masahiro YOSHIMURA

H3-12-106 ▶ Invited 16:30–17:05

Why Lattices and High Valence States. are Stabilized in Perovskite-Type Oxides by Madelung Lattice Site Potentials ?Masahiro YOSHIMURA

National Cheng Kung University

H3-12-107 ▶ Invited 17:05–17:40

Tuning Nb-doped SrTiO₃ surfaces and interfaces by chemical and electrical meansGunkel FELIX, Christoph BÄUMER, Regina DITTMANN

Forschungszentrum Juelich GmbH

H3-12-108 ▶ Invited 17:40–18:15

Construction of hierarchical oxide nanostructures for solar energy conversionJih-Jen WU, Jih-Sheng YANG, Shih-Yu CHEN

National Cheng Kung University

H3-12-009 18:15–18:30

Fabrication of ZnO/Co₃O₄ Heterojunction by Electrochemical DepositionYuzuki TOMITA, Masaya ICHIMURA

Nagoya Institute of Technology

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 13, 2019

Oral Session 7
Time 9:00–11:30 **Room** Miel-2

Chairpersons Yu SHIRATSUCHI, Jacobo SANTAMARIA

H3-13-K01 ▶ Keynote 9:00–10:00

Tailoring interface electronic states in tunnel devices based on correlated oxides
Jacobo SANTAMARIA
 Universidad Complutense

[Break 10:00–10:10]

H3-13-I02 ▶ Invited 10:10–10:45

Dynamic control of antiferromagnetic domain state based on magnetoelectric effect
Yu SHIRATSUCHI
 Osaka University

H3-13-003 10:45–11:00

Cross correlation of Ferromagnetism and Ferroelectricity in BiFeO₃
Shiro KAWACHI, Shin MIYAHARA, Toshimitsu ITO,
 Atsushi MIYAKE, Nobuo FURUKAWA, Jun-ichi YAMAURA,
 Masashi TOKUNAGA
 Tokyo Institute of Technology

H3-13-004 11:00–11:15

Epitaxial Growth of (111) ITO films for Top/bottom Electrodes of Ferroelectric Films
Kento SHIMAMOTO, Kohei MIURA, Junpei TANAKA,
 Daisuke KIRIYA, Takeshi YOSHIMURA, Atushi ASHIDA,
 Norifumi FUJIMURA
 Osaka Prefecture University

H3-13-005 11:15–11:30

Influence of Al₂O₃ ultrathin layer insertion at the interface of electrolyte and electrode in all-solid-state lithium batteries using anatase Nb-doped TiO₂ epitaxial thin films
Daisuke IMAZEKI¹, Kazunori NISHIO¹, Ryota SHIMIZU^{1,2},
 Taro HITOSUGI¹
¹Tokyo Institute of Technology, ²JST-PRESTO

December 13, 2019

Oral Session 8
Time 14:00–15:40 **Room** Miel-2

Chairpersons Hiroaki NISHIKAWA, Nobuyuki IWATA

H3-13-I06 ▶ Invited 14:00–14:35

Novel Functionalities in Atomically Controlled Oxide Heterostructures by Pulsed Laser Deposition
Guus RIJNDERS
 University of Twente

[Break 14:35–14:45]

H3-13-007 14:45–15:00

Influence of the film thickness on the formation of multilayer structures via spinodal decomposition in (Ti,V)O₂/TiO₂(100) films
Takahiro FUKUDA¹, Kensei TERASHIMA², Takanori WAKITA³,
 Takayoshi YOKOYA³, Yuji MURAOKA³
¹Okayama University, ²National Institute for Materials Science, ³Okayama University

H3-13-008 15:00–15:15

M-I Transition Control of VO₂ Thin Film by Excimer Laser assisted Metal Organic deposition (ELAMOD)
Tetsuo TSUCHIYA
 National Institute of Advanced Industrial Science and Technology (AIST)

H3-13-009 15:15–15:30

Growth and characterization of VO₂ thin films on hexagonal boron nitride
Hidekazu TANAKA¹, Mahito YAMAMOTO¹, Koji SHIGEMATSU²,
 Shodai ARITOMI³, Ryo NOUCHI^{4,5}, Teruo KANKI¹,
 Kenji WATANABE⁶, Takashi TANIGUCHI⁶,
 Yasukazu MURAKAMI², Shingo GENCHI¹
¹Osaka University, ²The Ultramicroscopy Research Center, Kyushu University, ³Department of Applied Quantum Physics and Nuclear Engineering, Kyusyu University, ⁴Osaka Prefecture University, ⁵JST PRESTO, ⁶National Institute for Materials Science

[Closing Remarks 15:30–15:40]

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 12, 2019

Poster Session

Time 14:00–15:30 Room Trade-0

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

H3-12-P01**Reactive sputtering deposition of distorted rutile-type MO_2 films ($M = Nb, Mo,$ and W)**Kohei FUJIWARA, Atsushi TSUKAZAKI
Tohoku University**H3-12-P02** **Fe_2O_3 -based pn junction solar cell fabricated by electrochemical deposition**Masaya ICHIMURA, Satoshi KOBAYASHI
Nagoya Institute of Technology**H3-12-P03****Synthesis of Stoichiometric La-doped $SrTiO_3$ from Bimetallic Complexes**Ebube OYEKA, Daichi OKA, Tomoteru FUKUMURA
Tohoku University**H3-12-P04****A Solution Route for Epitaxial Growth of β - Bi_2O_3 Nanostructures**Zaichun SUN¹, Daichi OKA¹, Tomoteru FUKUMURA^{1,2}
¹Department of Chemistry, Graduate School of Science, Tohoku University, ²WPI Advanced Institute for Materials Research and Core Research Cluster, Tohoku University**H3-12-P05****Metal-insulator transition in anti- $ThCr_2Si_2$ -type La_2O_2Bi via excess oxygen incorporation**Kota MATSUMOTO¹, Hideyuki KAWASOKO¹, Tomoteru FUKUMURA^{1,2}
¹Tohoku University, ²WPI-Advanced Institute for Materials Research and Core Research Cluster**H3-12-P06****Photorechargeable Properties of α - $Fe_2O_3/WO_3/FTO$ Triple-layer Coaxial Nanofibers**Taito KUMAMOTO
Kagoshima University**H3-12-P07****Application of Ce-doped $BiFeO_3$ Thin Film to Photoelectric Conversion in Photorechargeable Battery**Seiga UENO
Kagoshima University**H3-12-P08****Vertically Aligned Electrospun ITO Nanofibers and Their Application for Dye-sensitized Solar Cells**Kohei KOBAYASHI
Kagoshima University**H3-12-P09****Acceptor Doping of ZnO Films by NO Gas Decomposition on Heated Ir Wire Surface in a Catalytic Reaction-Assisted CVD**Kanji YASUI¹, Ryuta IBA¹, Koichiro OISHI², Hironori KATAGIRI², Ariyuki KATO¹¹Nagaoka University of Technology, ²National Institute of Technology, Nagaoka College**H3-12-P10****Total conductivity of yttria-stabilized lanthanum germanate fabricated by solid-state reaction method**Takaya TERAI¹, Kiyoshi KOBAYASHI^{1,2}, Tohru HIGUCHI¹, Tohru SUZUKI²¹Tokyo University of Science, ²National Institute for Materials Science**H3-12-P11****Low Temperature Growth of Rutile RuO_2 Epitaxial Thin Films by Pulsed Laser Deposition**Zainab FATIMA¹, Daichi OKA¹, Tomoteru FUKUMURA^{1,2}¹Department of Chemistry, Graduate School of Science, Tohoku University, ²WPI-Advanced Institute for Materials Research and Core Research Cluster, Tohoku University**H3-12-P12****Eliminating Carrier Compensating Defect in Doped ZnO Film by Zn Doping**Yasuji YAMADA, Yumika YAMADA, Rei SUGIURA, Shuhei FUNAKI
Shimane University**H3-12-P13****Impedance Measurements of $12CaO \cdot 7Al_2O_3 - 12SrO \cdot 7Al_2O_3$ Solid Solutions Prepared by High-pressure Synthesis**Masashi MIYAKAWA, Kiyoshi KOBAYASHI, Takashi TANIGUCHI
National Institute for Materials Science**H3-12-P14****Low Resistivity Doping-free Titanium Oxide Films Fabricated by Plasma-Assisted Deposition**Takahisa ICHINOHE, Hideki OHNO, Kouta SANO, Tadashi UEYAMA
National Institute of Technology, Tokyo College**H3-12-P15****Electric and Magnetic Properties at the Hetero-interface between $LaFeO_3$ and $SrTiO_3$** Hiroaki NISHIKAWA
Kindai University**H3-12-P16****Growth and Characterization of Tm Doped Gallium Oxide Films**Qixin GUO, Shunsuke MOTOMURA, Katsuhiko SAITO, Tooru TANAKA
Saga University

H3-12-P17

Aerosol-Sprayed Submicrometer Metal Oxide Spheres as Electromagnetic Resonators

Xizhe CHENG, Jianfang WANG
The Chinese University of Hong Kong

H3-12-P18

Magnetic and electric properties of near stoichiometric YbFe₂O₄ thin films fabricated by PLD using stoichiometric YbFe₂O₄ target with Fe₂O₃

Junpei TANAKA, Kouhei MIURA, Daisuke KIRIYA, Takeshi YOSHIMURA, Atsushi ASHIDA, Norifumi FUJIMURA
Osaka Prefecture University

H3-12-P19

Behaviors of physical property in multiferroic 0.7BaTiO₃-0.3Pr_{0.65}Ca_{0.35}MnO₃ core shell under laser light

Osami YANAGISAWA¹, Takashi FUJIMOTO², Kazuhiro KITAMURA³

¹Maritime Technology Department, National Institute of Technology, Yuge College, ²Electronic Mechanical Engineering Department, National Institute of Technology, Yuge College, ³Aichi University of Education

H3-12-P20

UV Light Detecting Properties of ZnO Nanorods Grown on Ion-plated Ga Doped ZnO Seed Layers by Chemical Bath Deposition

Tomoaki TERASAKO¹, Shohei OBARA¹, Suguru NAMBA¹, Naoto HASHIKUNI¹, Masakazu YAGI², Yutaka FURUBAYASHI³, Tetsuya YAMAMOTO³

¹Ehime University, ²National Institute of Technology (KOSEN), Kagawa College, ³Kochi University of Technology

H3-12-P21

Influence of Seed Layers on Structural and Morphological Properties of Nickel Hydroxide Nanowalls Grown by Chemical Bath Deposition

Tomoaki TERASAKO¹, Yutaka FURUBAYASHI², Tetsuya YAMAMOTO²

¹Ehime University, ²Kochi University of Technology

H3-12-P22

Systematic Control of Current Transport in Metal/Oxide Schottky Junctions Using Highly Uniform Layers of TaO_x

Atsushi FUKUCHI, Yusuke TSUTA, Masashi ARITA, Yasuo TAKAHASHI

Hokkaido University

H3-12-P23

Sol-gel Deposition and Direct Patterning of ZnO Thin Films

Koji ABE, Yasuhiro MORIMOTO
Nagoya Institute of Technology

H3-12-P24

Thin Iron Oxide Films Grown by Pulsed Laser Deposition

Valentin CRACIUN^{1,4}, M. KOMPITSAS², P. KORALLI², G. MOUSDIS², G. DORCIOMAN¹, Stefan IRIMICIUC¹, Bianca HODOROABA^{1,3}, D. CRACIUN¹, P. GAROI¹, M.D. DRACEA⁵, D PANTELICA⁵

¹National Institute for Laser, Plasma and Radiation Physics, ²National Hellenic Research, Foundation, Theor. and Phys./Chem. Institute, ³University of Bucharest, ⁴Extreme Light Infrastructure-Nuclear Physics, ⁵Horia Hulubei National Institute for Physics and Nuclear Engineering

H3-12-P25

Properties of Titanium Oxide/Titanium Composite Thin Films Formed on Transparent Plastic Substrates Using Magnetron DC Sputtering

Akira WATAZU, Tsutomu SONODA, Kei TERAOKA

National Institute of Advanced Industrial Science and Technology

H3-12-P26

Coupled Oscillation of VO₂ Layered Devices without Coupling Capacitor

Ryuta TOBE, Kunio OKIMURA, Md. Suruz MIAN

Tokai University

H3-12-P27

A Novel Floating Gate Memory with High Speed based on High-K Material

Lurong GAN

Fudan University

H3-12-P28

Magnetic Properties of Ferromagnetic Materials/*r*-plane oriented Cr₂O₃ Multilayers grown on YAlO₃(001) Substrate

Yukiya KUBOTA, Tomohiro TATENO, Hiroki KASHIMOTO, Takeru SATO, Nobuyuki IWATA

Nihon University

H3-12-P29

The Growth of YbFe₂O₄ Thin Films Prepared by Pulsed Laser Deposition Method with Different Energy Density at the Target Surface and Different Oxygen Partial Pressure

Kyoyua HIRAOKA, Takuya OKAMOTO, Takehiro TERAJI, Koudai SAKAMOTO, Syunpei YAMADA, Nobuyuki IWATA

Nihon University

H3-12-P30

Flexible Epitaxial Thin Films of Transparent Conducting Oxides

Akihiro HIRAOKA¹, Kohei FUJIWARA², Hiroaki NISHIKAWA³

¹Graduate School of Biology-Oriented Science and Technology, Kindai University, ²Tohoku University, ³Faculty of Biology-Oriented Science and Technology, Kindai University

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

H3-12-P31**Electronic Structure Characterization of Spinel NiCo₂X₄ (X = O and S): GGA and QSGW *ab-initio* Calculations**

Hasan AL RASYID¹, Masao OBATA^{1,2}, Indra PARDEDE¹,
Marleni WIRMAS¹, Takao KOTANI², Tatsuki ODA^{1,3}

¹Graduate School of Natural Science and Technology,
Kanazawa University, ²Institute of Science and Engineering,
Kanazawa University, ³Tottori University

H3-12-P32**In-plane Orientations of non c-axis Thin Films of Bi₂Sr₂CaCu₂O_{8+δ} and their Characterizations by scanning SQUID Microscopy**

Shunichi ARISAWA¹, Kazuhiro ENDO², Petre BADICA³

¹National Institute for Materials Science, ²Kanazawa
Institute of Technology, ³National Institute of Materials
Physics

H3-12-P33**Characteristics of High-energy H₂O Beam Generated by Catalytic Reaction for the Growth of Metal Oxide Thin Films**

Taro SAITO¹, Ryuta IBA¹, Abdul Manaf HASHIM²,
Kanji YASUI¹

¹Nagaoka University of Technology, ²MJIT, Universiti
Teknologi Malaysia

H3-12-P34**Adsorption of Amino Acids at TiO_x Particles on SrTiO₃ Surfaces Deposited Using Pulsed Laser Deposition**

Takuya IMI¹, Hiroaki NISHIKAWA²

¹Graduate School of Biology-Oriented Science and
Technology, Kindai University, ²Faculty of Biology-Oriented
Science and Technology, Kindai University

December 11–13, 2019

Symposium H-4

A3+ Lead-free Piezoelectric Materials and Applications

[Organizers]

Hajime NAGATA (Tokyo University of Science, Japan)
 Ichiro FUJII (University of Yamanashi, Japan)
 Satoshi WADA (University of Yamanashi, Japan)
 Yasuhiro YONEDA (Japan Atomic Energy Agency / Spring-8, Japan)
 Jing-Feng Li (Tsinghua University, China)
 Guorong Li (Shanghai Institute of Ceramics, China)
 Jae-Ho Jeon (Korea Institute of Materials Science, Korea)
 Shujun Zhang (University of Wollongong, Australia)
 Naratip Vittayakorn (King Mongkut's Institute of Technology
 Ladkrabang, Thailand)

December 11, 2019

Oral Session 3

Time 16:30–18:30 Room Miel-4

Chairpersons Takuya HOSHINA, Shujun ZHANG

H4-11-I01 ▶ Invited 16:30–17:00

Temperature- and Field-Dependent Local Structure in BaTiO₃ Materials Studied by Synchrotron X-Ray Absorption Spectroscopy

Rattikorn YIMNIRUN
 VISTEC

H4-11-I02 ▶ Invited 17:00–17:30

Structural Modeling Technique for Crystalline Metal Nanoparticles by X-ray Total Scattering Data

Satoshi HIROI¹, Koji OHARA², Osami SAKATA¹
¹National Institute for Materials Science, ²Japan Synchrotron Radiation Research Institute

H4-11-I03 ▶ Invited 17:30–18:00

Relationship between Structure and Physical Properties of Phosphate Glasses

Hirokazu MASAI¹, Shinji KOHARA², Yohei ONODERA³, Takahiro OHKUBO⁴, Akitoshi KOREEDA⁵
¹National Institute of Advanced Industrial Science and Technology, ²National Institute for Materials Science, ³Kyoto University, ⁴Chiba University, ⁵Ritsumeikan University

H4-11-004 18:00–18:15

Structural Phase Transitions and Improper Ferroelectricity in Aluminate-Sodalite-type Oxides

Hiroki TANIGUCHI¹, Chikako MORIYOSHI², Hiroki MORIWAKE³, Ichiro TERASAKI¹
¹Nagoya University, ²Hiroshima University, ³Japan Fine Ceramics Center

H4-11-005 18:15–18:30

Local structure analysis of (Na_{0.5}K_{0.45}Li_{0.05})NbO₃-based system with tetragonal structure

Yasuhiro YONEDA
 Japan Atomic Energy Agency

December 12, 2019

Oral Session 4

Time 9:00–11:00 Room Miel-4

Chairpersons Jing-Feng LI, Satoshi WADA

H4-12-I01 ▶ Invited 9:00–9:30

Ferroelectric Structural Phase Transition and Staggered Phase Transition in Lead-Free Piezoelectric KNN

Takayuki MATSUOKA, Masato YAMAZAKI
 NGK SPARK PLUG CO., LTD.

H4-12-I02 ▶ Invited 9:30–10:00

The electric fatigue resistance and temperature-dependent piezoresponse of KNN-based ceramics

Jiwei ZHAI
 Tongji University

H4-12-I03 ▶ Invited 10:00–10:30

Lead-free Potassium-Sodium Niobate Ceramics: From Property to Devices

Jiagang WU
 Sichuan University

H4-12-004 10:30–10:45

Fabrication and piezoelectric properties of (K_{0.5}Na_{0.5})NbO₃ single crystals by solid-state crystal growth method

Ichiro FUJII, Shintaro UENO, Satoshi WADA
 University of Yamanashi

H4-12-005 10:45–11:00

Composition design, structure and properties of niobate-based ceramics

Dong YANG
 Tsinghua University

December 12, 2019

Oral Session 6

Time 16:30–18:45 Room Miel-4

Chairpersons Yasuhiro YONEDA, Rattikorn YIMNIRUN

H4-12-I06 ▶ Invited 16:30–17:00

AgNbO₃-based Lead-free Antiferroelectrics for Energy Storage Applications

Jing-Feng LI
 Tsinghua University

H4-12-I07 ▶ Invited 17:00–17:30
Crystal Structures and Dielectric Properties of Perovskite-Type Mixed-Anion Compound
 Takuya HOSHINA, Hiroaki TAKEDA, Takaaki TSURUMI
 Tokyo Institute of Technology

H4-12-I08 ▶ Invited 17:30–18:00
Bismuth Ferrite based solid solution piezoelectric/ferroelectric materials and their applications
 Zhenxiang CHENG
 University of Wollongong

H4-12-009 18:00–18:15
Electromechanical and electrocaloric properties of NaNbO_3 and $(\text{Pb,L a})(\text{Zr,Ti})\text{O}_3$ ceramics
 Hiroshi MAIWA, Atsushi SAKURAI, Yugeng LIU
 Shonan Institute of Technology

H4-12-I10 ▶ Invited 18:15–18:45
Improve photocatalysis property of ferroelectric oxides
 Yaodong YANG, Bian YANG
 Xi'an Jiaotong University

December 13, 2019

Oral Session 7

Time 9:00–11:00 Room Miel-4

Chairpersons Naratip VITTAYAKORN, Hajime NAGATA

H4-13-I01 ▶ Invited 9:00–9:30
Processing and Properties of $(\text{Bi}_{1/2}\text{K}_{1/2})\text{TiO}_3$ -based Piezoelectric Ceramics
 Manabu HAGIWARA, Makoto ITO, Shinobu FUJIHARA
 Keio University

H4-13-I02 ▶ Invited 9:30–10:00
Large electrostrain response in Mn-modified $0.94(\text{Bi}_{0.5}\text{Na}_{0.5})\text{TiO}_3$ - 0.06BaTiO_3 lead-free piezoceramics
 Danyang WANG, Le ZHANG, Haoyu WANG
 UNSW Sydney

H4-13-I03 ▶ Invited 10:00–10:30
Combustion Synthesis and Properties of $0.94\text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3$ - $0.06\text{Ba}_{0.85}\text{Ca}_{0.15}\text{Ti}_{0.90}\text{Zr}_{0.10}\text{O}_3$ ceramics doped with $\text{Bi}_2\text{FeCrO}_6$
 Theerachai BONGKARN
 Naresuan University

H4-13-004 10:30–10:45
Perovskite $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$: Potential Family of Peculiar Lead-free Electrostrictors
 Jie YIN
 Sichuan University

H4-13-005 10:45–11:00
AC Poling Treatment in Grain-oriented BT-BNT Piezoceramics
 Satoshi WADA
 University of Yamanashi

December 13, 2019

Oral Session 8

Time 14:00–15:30 Room Miel-4

Chairpersons Ichiro FUJII, Theerachai BONGKARN

H4-13-I06 ▶ Invited 14:00–14:30
NBT and KNN based textured and non-textured lead free ceramics
 Shujun ZHANG¹, Xiaoyi GAO^{1,2}, Hua HAO², Hanxing LIU², Nannan DONG², Peng LI³, Jiwei ZHAI³
¹University of Wollongong, ²Wuhan University of Technology, ³Tongji University

H4-13-I07 ▶ Invited 14:30–15:00
Conceivable strategies for making Lead-free piezoelectrics practical
 Wook JO
 Ulsan National Institute of Science and Technology

H4-13-008 15:00–15:15
A Template-free Salt-flux-assisted Synthesis of Tetragonal BaTiO_3 Nanowires and Its Piezoelectric Response for Flexible Nanogenerators
 Thitirat CHAROONSUK¹, Saichon SRIPHAN¹, Chanisa NAWANIL², Narong CHANLEK³, Wanwilai VITTAYAKORN¹, Utchawadee PHARINO¹, Naratip VITTAYAKORN¹
¹King Mongkut's Institute of Technology Ladkrabang, ²Udon Thani Rajabhat University, ³Synchrotron Light Research Institute

H4-13-009 15:15–15:30
Dielectric Anomalies Suppression of Co-doped BaZrO_3 with Ultrahigh Q-factor
 Phieraya PULPHOL¹, Rangson MUANGHLUA¹, Naratip VITTAYAKORN¹, Taras KOLODIAZHNYI², Wanwilai VITTAYAKORN¹
¹King Mongkut's Institute of Technology Ladkrabang, ²National Institute for Material Science

December 12, 2019

Poster Session

Time 14:00–15:30 Room Trade-0

H4-12-P01

Quenching Effects for Depolarization Temperature on $(\text{Bi}_{0.5}\text{Na}_{0.5})\text{TiO}_3\text{-ZnO}$ Ceramics by Controlling the Firing Conditions

Yuto ITAKURA, Yuka TAKAGI, Hajime NAGATA, Tadashi TAKENAKA
Tokyo University of Science

H4-12-P02

Preparation and Characterization of Graphene/ $\text{Bi}(\text{Fe},\text{Mn})\text{O}_3$ Structure on SrRuO_3 -buffered SrTiO_3 Substrate

Seiji NAKASHIMA, Sho YAMAGATA, Yakumo FUCHIWAKI, Satoru SUZUKI, Hironori FUJISAWA
University of Hyogo

H4-12-P03

Fabrication of 111-Oriented BaTiO_3 Ceramics by a High-Magnetic-Field-Assisted Electrophoretic Deposition Method with Co-Existing Hexagonal-Tetragonal Phases of BaTiO_3 Powders

Hari Shankar MALLIK, Sangwook KIM, Ichiro FUJII, Shintaro UENO, Satoshi WADA
University of Yamanashi

H4-12-P04

High-Power Piezoelectric Properties of Mn-doped $(\text{Bi}_{0.5}\text{Na}_{0.5})\text{TiO}_3\text{-(Bi}_{0.5}\text{K}_{0.5})\text{TiO}_3\text{-BaTiO}_3$ based ceramics at MPB composition

Tomoya UENO, Yuka TAKAGI, Hajime NAGATA, Tadashi TAKENAKA
Tokyo University of Science

H4-12-P05

High-Power Piezoelectric Characteristics of MnCO_3 and CuO Co-Doped $\text{Ba}(\text{Zr},\text{Ti})\text{O}_3\text{-(Ba,Ca)TiO}_3$ Ceramics

Takuo TOMINAGA, Yuka TAKAGI, Hajime NAGATA, Tadashi TAKENAKA
Tokyo University of Science

H4-12-P06

The quenching effects for depolarization temperature of $(\text{Bi}_{0.5}\text{Na}_{0.5})\text{TiO}_3$ ceramics with various dopants

Koutaro EGUCHI, Yuka TAKAGI, Hajime NAGATA, Tadashi TAKENAKA
Tokyo University of Science

H4-12-P07

Investigation of Mn-Nb Co-doped Barium Titanate Ceramics for DC-bias free Dielectrics

Piyush SAPKOTA, Ichiro FUJII, Shintaro UENO, Satoshi WADA
University of Yamanashi

H4-12-P08

Structural and Piezoelectric Properties of Lead-free Piezoelectric Ceramics in the $\text{BaTiO}_3\text{-BiFeO}_3$

Hyunwook NAM, Ichiro FUJII, Sangwook KIM, Shintaro UENO, Satoshi WADA
University of Yamanashi

H4-12-P09

Structure analysis of $(\text{Ca},\text{Ba})\text{Nb}_2\text{O}_5$ ceramic powder from high-energy X-ray diffraction

Yasuhiro YONEDA
Japan Atomic Energy Agency

H4-12-P10

The BaTiO_3 /PDMS Composite Film Modified with $\text{Ti}_{0.8}\text{O}_2$ Nanosheets and Silver Nanopowders for Flexible Nanogenerators

Naratip VITTAYAKORN, Saichon SRIPHAN, Thitirat CHAROONSUK, Tosapol MALUANGNONT
King Mongkut's Institute of Technology Ladkrabang

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 11–13, 2019

Symposium H-5Intelligent Material Processes with Low
Environmental Load and Energy Consumption

[Organizers]

Nobuhiro MATSUSHITA (Tokyo Institute of Technology)
 Tomoaki WATANABE (Meiji University)
 Hajime WAGATA (Meiji University)
 Yung-Jung HSU (National Chiao Tung University)
 Ferry ISKANDAR (Institute of Technology Bandung)

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December 11, 2019

Oral Session 3

Time 16:30–18:35 Room Mont-5

Chairpersons Ken-ichi KATSUMATA,
 Tomoaki WATANABE

Opening
 Nobu Matsushita (Tokyo Tech)
 16:30–16:35

H5-11-K01 ▶ Keynote 16:35–17:15

Semiconductor Nanoheterostructures for
 Photoconversion Applications

Yung-Jung HSU
 National Chiao Tung University

H5-11-I02 ▶ Invited 17:15–17:40

Behavior of Photogenerated Charge Carriers on Powder
 Photocatalysts

Akira YAMAKATA
 Toyota Technological Institute

Break
 17:40–17:50

H5-11-003 17:50–18:05

Hydrothermal Synthesis of Rutile-type Titania Crystals
 with Pseudocubic Shapes

Makoto KOBAYASHI¹, Hideki KATO², Minoru OSADA¹,
 Masato KAKIHANA²

¹Institute of Materials and Systems for Sustainability,
 Nagoya University, ²Institute of Multidisciplinary Research
 for Advanced Materials, Tohoku University

H5-11-004 18:05–18:20

One-pot synthesis of (B/A)-TiO₂ nanosheet/Carbon dot
 heterostructure for enhanced visible-light-photocatalysis

Sovann KHAN¹, Norihiro SUZUKI¹, Kazuya NAKATA²,
 Chiaki TERASHIMA¹, Akira FUJISHIMA¹,
 Ken-ichi KATSUMATA¹

¹Tokyo University of Science, ²Tokyo University of
 Agriculture and Technology

H5-11-005 18:20–18:35

TiO₂ Nanowire-Supported Sulfide Hybrid Photocatalysts
 for Durable Solar Hydrogen Production

Ping-Yen HSIEH

Department of Materials Science and Engineering, National
 Chiao Tung University

December 12, 2019

Oral Session 4

Time 9:00–11:30 Room Trade-2

Chairpersons Hajime WAGATA, Sayaka YANAGIDA

H5-12-001 9:00–9:15

Design of Full-Spectrum-Drive Photoelectrodes for
 Water Splitting

Yu Ting WANG

Material Science and Engineering of Chiao Tung University

H5-12-002 9:15–9:30

Tin Sulfide Colloidal Nanocrystals: Synthesis and
 Characterization

Retno MIRANTI¹, Satria Zulkarnaen BISRI^{2,1},
 Yoshihiro IWASA^{2,3}, Nobuhiro MATSUSHITA¹

¹Tokyo Institute of Technology, ²RIKEN Center for Emergent
 Matter Science (CEMS), ³The University of Tokyo

H5-12-003 9:30–9:45

Facet Effect of Au@CdS Yolk@Shell Nanocrystals on
 Photocatalytic Hydrogen Production

Yi-An CHEN, Yung-Jung HSU

Department of Materials Science and Engineering, National
 Chiao Tung University

H5-12-004 9:45–10:00

Significant Performance of Ammonia Borane
 Dehydrogenation Using Au@Cu₂O Core@Shell
 Nanocrystals

Mei Jing FANG

National Chiao Tung University

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

H5-12-005 10:00–10:15

Preparation of Au@Cu₂O Core-shell Particles on Rutile Rods using Step-by-step Photocatalytic Deposition and Investigation of their Photocatalytic Cr(IV) Reduction Ability
Sayaka YANAGIDA, Takumi YAJIMA, Takahiro TAKEI, Nobuhiro KUMADA
University of Yamanashi

[Break
10:15–10:25]

H5-12-I06 ▶ Invited 10:25–10:50

Microwave-assisted Synthesis of Carbon Nanostructured Materials and Its Physical Properties
Ferry ISKANDAR^{1,2}, Fitri A. PERMATASARI¹
¹Institut Teknologi Bandung, ²Research Center for Nanosciences and Nanotechnology

H5-12-I07 ▶ Invited 10:50–11:05

Solution Plasma and Hetero-Graphene
SANGWOO CHAE^{1,3}, PHUWADEJ PORNAROONTHAM^{1,3}, NAGAIHIRO SAITO^{1,2,3,4}
¹Department of Chemical Systems Engineering, Graduate School of Engineering, Nagoya University, ²Conjoint Research Laboratory in Nagoya University, Shinshu University, ³Japan Science and Technology Corporation (JST), Open Innovation Platform with Enterprises, Research Institute and Academia (OPERA), ⁴Japan Science and Technology Corporation (JST), Strategic International Collaborative Research Program (SICORP)

H5-12-008 11:05–11:30

Preparation of Nanosheets by Using Ionic Liquids
Ken-ichi KATSUMATA¹, Tetsuya YAMADA², Yuta KUBOTA³, Yuki MAKINOSE⁴, Norihiro SUZUKI¹, Kazuya NAKATA⁵, Chiaki TERASHIMA¹, Nobuhiro MATSUSHITA³, Akira FUJISHIMA¹
¹Tokyo University of Science, ²Kanagawa Institute of Industrial Science and Technology, ³Tokyo Institute of Technology, ⁴Shimane University, ⁵Tokyo University of Agriculture and Technology

December 12, 2019

Oral Session 5
Time 14:00–16:00 **Room** Trade-2

 Chairpersons Ferry ISKANDAR, Yoshitake MASUDA
H5-12-I09 ▶ Invited 14:00–14:25

Intelligent Material Processes with Low Environmental Load and Energy Consumption for Nanostructuring of Metal Oxides -Gas/Chemical Sensors with SnO₂, TiO₂, ZnO-
Yoshitake MASUDA
National Institute of Advanced Industrial Science and Technology (AIST)

H5-12-010 14:25–14:40

Liquid-phase Synthesis of Pt-loaded Y₂WO₆:Eu³⁺ Phosphor Particles for Hydrogen Gas Sensing
Hong YE, Manabu HAGIWARA, Shinobu FUJIHARA
Keio University

H5-12-011 14:40–14:55

Preparation and Gas Sensor Characteristics of Ni-Zn Ferrite Thin Film Deposited on Porous Silicon
Hiroki ISHIGAMI
Department of Electronics Science, Shizuoka University

[Break
14:55–15:00]

H5-12-012 15:00–15:15

Low environmental loading process: Spin spray for thin film deposition of functional metal oxides
Hwai En LIN, Yuta KUBOTA, Nobuhiro MATSUSHITA
Tokyo Institute of Technology

H5-12-013 15:15–15:30

Preparation of transparent conductive ZnO film by Non-Seed CBD method
Naoya SHIOIRI, Hajime WAGATA
Meiji University

H5-12-014 15:30–15:45

Resistive Switching Properties of Liquid Phase Deposited Cerium Oxide Films
Yuta KUBOTA, Tetsuya FURUKAWA, Nobuhiro MATSUSHITA
Tokyo Institute of Technology

H5-12-015 15:45–16:00

Liquid-phase Synthesis and Morphology Control of Ferroelectric BiFeO₃ Particles for Stress Sensing Applications
Kohei YOSHIYAMA, Manabu HAGIWARA, Shinobu FUJIHARA
Keio University

December 12, 2019

Oral Session 6
Time 16:30–18:25 **Room** Trade-2

 Chairpersons Masamoto TAFU, Hiroyuki MUTO
H5-12-K16 ▶ Keynote 16:30–17:10

Intelligent Material Processes with Ceramic Nanocrystals
Minoru OSADA
Nagoya University

H5-12-I17 ▶ Invited 17:10–17:35
Advanced Composite Particles Integration Process via Electrostatic Assembly Method
 Hiroyuki MUTO, Atsushi YOKOI, Wai Kian TAN, Go KAWAMURA, Atsunori MATSUDA
 Toyohashi University of Technology

Break
 17:35–17:45

H5-12-I18 ▶ Invited 17:45–18:10
Development of Functional Coatings Showing Paradoxical Surface Wetting/Dewetting Properties
 ATSUSHI HOZUMI
 AIST

H5-12-019 18:10–18:25
Development of novel sol-gel based surface initiator layers for surface-initiated ATRP (SI-ATRP)
 Tomoya SATO¹, Gary J. DUNDERDALE^{1,2}, Chihiro URATA¹, Atsushi HOZUMI¹
¹National Institute of Advanced Industrial Science and Technology (AIST), ²Department of Chemistry, University of Sheffield

December 13, 2019

Oral Session 7

Time 9:00–11:30 Room Mont-5

Chairpersons Yuta KUBOTA, Naonori SAKAMOTO

H5-13-I01 ▶ Invited 9:00–9:25
Bioaccumulation and biomineralization on a radural teeth of chiton, *Acanthopreura japonica*.
 Chiya NUMAKO
 Chiba University

H5-13-I02 ▶ Invited 9:25–9:50
Effect of hybridization on reactivity of dicalcium phosphate dihydrate (DCPD) by apatites nano-particles for solidification of fluoride ions
 Masamoto TAFU, Natsuki OKAJIMA, Takeshi TOSHIMA, Saori TAKAMATSU
 National Institute of Technology, Toyama College

H5-13-003 9:50–10:05
Effective Tellurium Recovery from Bi-Sb-Te Intermetallic Solid Materials by Wet Mechanochemical Technique
 Ryo SASAI¹, Takuya FUJIMURA¹, Kazushi URABE¹, Takuya SANO²
¹Shimane University, ²ARBIZ Corporation

Break
 10:05–10:20

H5-13-I04 ▶ Invited 10:20–10:45
New Type Solid-State Reaction, Water-Assisted Solid-State Reaction
 Kenji TODA
 Niigata University

H5-13-005 10:45–11:00
Cement sludge recycling system using sodium gluconate
 Daiki ATARASHI¹, Hiroshi FURUI¹, Eiji SUNADA³, Eiichi KATSUBE⁴, Yuichi TSUKADA⁵
¹Shimane University, ²Hiroshima Area Concrete Cooperative Association, ³Maruse, ⁴Kitagawa Corporation, ⁵DKK-TOA Corporation

H5-13-006 11:00–11:15
Controlled Fabrication of Textured and Porous Ca₃Co₄O₉ Ceramics and Their Thermoelectric Property
 Rina SHIMONISHI, Manabu HAGIWARA, Shinobu FUJIHARA
 Keio University

H5-13-007 11:15–11:30
Growth and characterization of Li_xLa_{(1-x)/3}NbO₃ single crystals by TSFZ method
 MD SHAHAJAN ALI
 CCST, University of Yamanashi

December 13, 2019

Oral Session 8

Time 14:00–16:00 Room Work-5

Chairpersons Chiya NUMAKO, Akifumi MATSUDA

H5-13-I08 ▶ Invited 14:00–14:25
Preparation of Ultrathin Nanosheet pn-Junction and Photocatalytic Activity
 Shintaro IDA, Keisuke AWAYA
 Kumamoto University

H5-13-009 14:25–14:40
Solution-Phase Ligand-Exchange of Lead Sulfide Colloidal Quantum Dot for Facile Thick Film Fabrication
 Ricky Dwi SEPTIANTO^{1,2}, Satria Zulkarnaen BISRI^{1,2}, Nobuhiro MATSUSHITA², Yoshihiro IWASA^{1,3}
¹RIKEN CEMS, ²Tokyo Institute of Technology, ³The University of Tokyo

H5-13-010 14:40–14:55
Room-temperature epitaxy and optoelectronic properties of heavily doped Ni_{1-x}Fe_xO thin films
 Akifumi MATSUDA¹, Seo OKKYUN², Osami SAKATA^{2,1}, Mamoru YOSHIMOTO¹
¹Tokyo Institute of Technology, ²National Institute for Materials Science

Break
 14:55–15:05

H5-13-I11 ▶ Invited 15:05–15:30

Growth Mechanism of mist CVD

 Toshiyuki KAWAHARAMURA^{1,2,3}, Li LIU^{1,2,3},
 Phimolphan RUTTHONGJAN², Shota SATO², Mariko UEDA²,
 Tatsuya YASUOKA², Yuki TAGASHIRA², Tamako OZAKI²,
 Yuna ISHIKAWA¹, Miyabi FUKUE¹, Giang T. DANG^{1,2,3}
¹School of Sys. Eng., Kochi University of Technology, ²Eng.
 Course, Graduate School of Engineering, Kochi University
 of Technology, ³Center for Nanotechnology, Res. Inst.,
 Kochi University of Technology

H5-13-012 15:30–15:45

Development of Electrostatic LSMCD, and Preparation and Characterization of Alumina Thin Film

 Takuma SUZUKI, Takahiko KAWAGUCHI,
 Naonori SAKAMOTO, Hisao SUZUKI, Naoki WAKIYA
 Department of Electrics and Materials Science, Shizuoka
 University

H5-13-013 15:45–16:00

Analysis of ferroelectric thin films by cross sectional AFM

 Naonori SAKAMOTO, Satoshi MIYAZAKI, Kohei KASAMI,
 Takahiko KAWAGUCHI, Naoki WAKIYA, Hisao SUZUKI
 Shizuoka University

December 13, 2019

Oral Session 9

Time 16:30–18:25 Room Work-5

Chairpersons Shitaro IDA, Shintaro YASUI

H5-13-I14 ▶ Invited 16:30–16:55

Development of high power blue diode laser for additive manufacturing of pure copper

 Masahiro TSUKAMOTO
 Joining and Welding Research Institute, Osaka University

H5-13-015 16:55–17:10

Ultra-high Rate Performance of LiCoO₂ Cathode Thin Film Battery

 Shintaro YASUI¹, Sou YASUHARA¹, Takashi TERANISHI²,
 Yumi YOSHIKAWA², Tomoyasu TANIYAMA³, Mitsuru ITOH¹
¹Tokyo Institute of Technology, ²Okayama University,
³Nagoya University

H5-13-016 17:10–17:25

Preparation of YSZ Thin Film on Through-Hole-Type Porous Silicon

 Hiroki NAKANE
 Department of Electronics Science, Shizuoka University

 Break
 17:25–17:40

H5-13-017 17:40–17:55

Development of Novel Dynamic Aurora PLD which Enables *in-situ* Observation of Epitaxial Growth of Ceramic Thin Films

 Mayu YOSHIDA
 Department of Electronics Science, Shizuoka University

H5-13-018 17:55–18:10

Preparation of Ca₃Co₄O₉ Thin Film by Dynamic Aurora PLD

 Tetsunari TANADA, Takahiko KAWAGUCHI,
 Naonori SAKAMOTO, Hisao SUZUKI, Naoki WAKIYA
 Department of Electronics and Materials Science, Shizuoka
 University

H5-13-019 18:10–18:25

Perpendicular Magnetic Anisotropy in Nickel Ferrite Thin Films

 Keisuke TAKASHIMA¹, Nipa DEBNATH¹,
 Takahiko KAWAGUCHI¹, Naonori SAKAMOTO¹,
 Kazuo SHINOZAKI², Hisao SUZUKI¹, Naoki WAKIYA¹
¹Shizuoka University, ²Tokyo Tech

Closing

Nobuhiro Matsushita (Tokyo Tech)

18:25~

December 13, 2019

Poster Session

Time 19:00–20:30 Room Trade-0

H5-13-P01

Synthesis of Xonotlite in Cement-Silica-Portlandite system

 Yuta MORIMOTO¹, Daiki ATARASHI¹, Kouichi IMASAWA²
¹Shimane University, ²Sumitomo Metal Mining Siporex

H5-13-P02

Effect of calcium nitrite on hydration of blast furnace slag

 Shuya OSAKI¹, Daiki ATARASHI¹, Hyeonjin SONG¹,
 Yuhji SUDOH²
¹Shimane University, ²Nissan Chemical Co., Ltd

H5-13-P03

Effect of Alkanolamine on reaction of 4CaO·Al₂O₃·Fe₂O₃

 Hyeonjin SONG¹, Daiki ATARASHI², Yoshifumi HOSOKAWA³,
 Miho MIYAKAWA⁴
¹Shimane University, ²Shimane University, ³TAIHEIYO
 CEMENT CORPORATION, ⁴GCP Chemicals CO.,LTD

H5-13-P04**Highly Cationic Nitrogen-doped Graphene to Enhance Electric Properties via Solution Plasma**

SANGWOO CHAE^{1,4}, GASIDIT PANOMSUWAN², NAGAHIRO SAITO^{1,3,4,5}

¹Department of Chemical Systems Engineering, Graduate School of Engineering, Nagoya University, ²Department of Materials Engineering, Faculty of Engineering, Kasetsart University, ³Conjoint Research Laboratory in Nagoya University, Shinshu University, ⁴Japan Science and Technology Corporation (JST), Open Innovation Platform with Enterprises, Research Institute and Academia (OPERA), ⁵Japan Science and Technology Corporation (JST), Strategic International Collaborative Research Program (SICORP)

H5-13-P05**Synergistic Effect of Electrical Properties of Cationic Nitrogen-Doped Carbon and Carbon Nanotubes Composites Synthesized via Plasma Solution.**

Sangwoo CHAE^{1,3}, Takumi YANA¹, Nagahiro SAITO^{1,2,3,4}

¹Department of Chemical Systems Engineering, Graduate School of Engineering, Nagoya University, ²Conjoint Research Laboratory in Nagoya University, Shinshu University, ³Japan Science and Technology Corporation (JST), Open Innovation Platform with Enterprises, Research Institute and Academia (OPERA), ⁴Japan Science and Technology Corporation (JST), Strategic International Collaborative Research Program (SICORP)

H5-13-P06**Investigation of N-doped Carbon Dots Synthesized by Solution Plasma for Detection of Nitro Aromatic Molecules**

Kyusung KIM^{1,3}, Junmo MOON¹, Nagahiro SAITO^{1,2,3,4}

¹Department of Chemical Systems Engineering, Graduate School of Engineering, Nagoya University, ²Conjoint Research Laboratory in Nagoya University, Shinshu University, ³Japan Science and Technology Corporation (JST), Open Innovation Platform with Enterprises, Research Institute and Academia (OPERA), ⁴Japan Science and Technology Corporation (JST), Strategic International Collaborative Research Program (SICORP)

H5-13-P07**Analyzing properties of nitrogen, boron and nitrogen-boron doped few-layer graphene coated copper nanoparticles synthesized by solution plasma for oxygen reduction reaction catalyst**

Phu Quoc PHAN¹, Kyusung KIM^{1,3}, Yukihiro MUTA^{1,3}, Mongkol TIPPLOOK^{1,3}, Sangwoo CHAE^{1,3}, Nagahiro SAITO^{1,2,3,4}

¹Department of Chemical Systems Engineering, Graduate School of Engineering, Nagoya University, ²Conjoint Research Laboratory in Nagoya University, Shinshu University, ³Japan Science and Technology Corporation (JST), Open Innovation Platform with Enterprises, Research Institute and Academia (OPERA), ⁴Japan Science and Technology Corporation (JST), Strategic International Collaborative Research Program (SICORP)

H5-13-P08**Synthesis of nitrogen-oxygen-codoped nanocarbons via solution plasma process and nitridation for CO₂ adsorption**

PHUWADEJ PORNAROONTHAM^{1,4}, GASIDIT PANOMSUWAN², NAGAHIRO SAITO^{1,3,4,5}

¹Department of Chemical Systems Engineering, Graduate School of Engineering, Nagoya University, ²Department of Materials Engineering, Faculty of Engineering, Kasetsart University, ³Conjoint Research Laboratory in Nagoya University, Shinshu University, ⁴Japan Science and Technology Corporation (JST), Open Innovation Platform with Enterprises, Research Institute and Academia (OPERA), ⁵Japan Science and Technology Corporation (JST), Strategic International Collaborative Research Program (SICORP)

H5-13-P09**Development of fabrication process for BaTaO₂N photoanodes using roll press method and calcination**

Mizuki ITO, Tomoaki WATANABE
Meiji University

H5-13-P10**Development of fabrication method for layered photoanodes by using roll press method**

Mai IJIMA, Tomoaki WATANABE
Meiji University

H5-13-P11**Synthesis and Evaluation of Sphere-like CuO Films on Conductive Substrates by Direct Annealing Method**

Ryo NISHIDA, Tomoaki WATANABE
Meiji University

H5-13-P12**Cu_{2-x}O-Fe₂O₃ Composite Films Prepared By Low Temperature Solution Process**

Kazuya SHIMADA, Hwai-En LIN, Yuta KUBOTA, Nobuhiro MATSUSHITA
Tokyo Institute of Technology

H5-13-P13**Growth and characterization of LiCoO₂ single crystals by Traveling Solvent Floating Zone(TSFZ) technique using tilted-mirror type furnace.**

Ruma PARVIN
University of Yamanashi

H5-13-P14**Synthesis of Nano LiCoO₂ by Water-Assisted Solid-State Reaction Method**

Tsukasa HOSHI
Graduate School of Niigata University

H5-13-P15

Electrochemical properties of $\text{Cu}_{2-x}\text{O}-\alpha\text{Fe}_2\text{O}_3$ composite film for supercapacitor

Michihiko UEMURA

Tokyo Institute of Technology

H5-13-P16

Optimization of doping amount of upconversion phosphor by parallel synthesis using complex gelation method

Kohei KASUYA¹, Sayaka TAMURA², Yasushi SATO³, Makoto KOBAYASHI⁴, Hideki KATO⁵, Masato KAKIHANA⁵, Koji TOMITA¹

¹Tokai University, ²Kanagawa University, ³Okayama University of Science, ⁴Nagoya University, ⁵Tohoku University

H5-13-P17

A New Low-Temperature Synthesis of $\text{K}_2\text{NbO}_3\text{F}$ with NH_4F as a Fluorinating Agent

Masaru WATANABE

Graduate School of Science and Technology, Niigata University

H5-13-P18

Ca - Al - O: (Eu, Nd) phosphors synthesized on mortar hardened body

Keiji KOMATSU¹, Tetsuro KIMURA¹, Atsushi NAKAMURA², Hidetoshi SAITOH¹

¹Nagaoka University of Technology, ²Chubu Chelest

H5-13-P19

Pure Copper Film Welding with Near Infrared and Blue Diode Lasers

Kento MORIMOTO¹, Masahiro TSUKAMOTO², Shin-ichiro MASUNO², Yuji SATO³, Kazuyuki AZUMI⁴, Yoshihiko HAYASHI⁴

¹Graduate School of Engineering, Osaka University, ²Joining and welding research institute, Osaka University, ³Japan Atomic Energy Agency, ⁴Osaka Fuji Corporation

H5-13-P20

Formation of aligned peptide films by blade coating and their structural analysis

Kazunori MOTAI

Tokyo Institute of Technology

H5-13-P21

Fabrication of Bioactive and Antibacterial Nanostructured Surface on Ti-based BMG Surface by Hydrothermal-Electrochemical Process

Nobuhiro MATSUSHITA

Tokyo Institute of Technology

H5-13-P22

Effect of crystallinity of FAp (fluorapatite) on adsorption of ammonia gas

Aoi IWAORI

National Institute of Technology, Toyama College

H5-13-P23

Analytical Research on Preservation and Restoration Method of Excavated Ancient Coins

Yuko NISHIMOTO¹, Yuki AOYANAGI¹, Shinya NAGASAKO²

¹Kanagawa Univ., ²Tokyo metropolitan Archaeological Center

H5-13-P24

Simultaneous Formation Process of $\text{Ti}_3\text{SiC}_2/\text{TiC}$ Composite Films from Their Elemental Materials

Tsutomu SONODA, Akira WATAZU, Setsuo NAKAO

National Institute of Advanced Industrial Science and Technology

H5-13-P25

Improvement Of Packing Structure Of Green Body Via Electrostatic Nano-Assembly Technique

Ryota OGASAWARA

Toyohashi University of Technology

H5-13-P26

Orientation controlled room-temperature growth of ZnO (0001) thin films on atomic-step patterned flexible polymer substrates

Tomoaki OGA¹, Hiroyuki MORITA¹, Satoru KANEKO^{2,1}, Akifumi MATSUDA¹, Mamoru YOSHIMOTO¹

¹Tokyo Institute of Technology, ²Kanagawa Institute of Industrial Science and Technology

H5-13-P27

Preparation of Zinc Oxynitride Thin Films by a Solution Process and Subsequent Nitridation

Shota EBARA, Hajime WAGATA

Meiji University

H5-13-P28

Growth of ZnO Mesocrystals Using Mixed Solvents of Choline Chloride – Urea Deep Eutectic Solvent and Ethylene Glycol

Hajime WAGATA¹, Eriko NAKASHIMA¹, Motoki ASAGA¹, Masaru TADA², Kunio YUBUTA³

¹Meiji University, ²Tokyo Institute of Technology, ³Tohoku University

Cluster I

Biopolymers

Symposium

- I-1** Bio-based Polymers
- I-2** Environmentally Degradable Polymers
- I-3** Biodegradable Polymers for Biomedical Applications

December 13, 2019

Symposium I-1

Bio-based Polymers

[Organizer]

Hideki ABE (RIKEN CSRS)

December 13, 2019

Oral Session 7

Time 9:00–11:20 Room Mont-1

Chairpersons Hideki ABE, Takeharu TSUGE

I112-13-001 9:00–9:15

Development of Heat-resistant Polymeric Materials from Bio-based Chemicals

Hideki ABE

RIKEN Center for Sustainable Resource Science

I112-13-K02 ▶ Keynote 9:15–9:45

Controlled/Living Polymerization of Functional Styrenes from Natural Resources

Kotaro SATOH

Tokyo Institute of Technology

I112-13-003 9:45–10:00

Fabrication of Multiple Parallel Gel Filaments by Applying Shear to Polymer Assembly

Yuriko TAKAYAMA, Norihiro KATO

Utsunomiya University

I112-13-I04 ▶ Invited 10:00–10:20

Protease-catalyzed Polymerization for Synthesis of Polypeptides with Specific Sequence Motifs

 Kousuke TSUCHIYA^{1,2}, Keiji NUMATA^{1,2}
¹RIKEN, ²JST-ERATO

I112-13-I05 ▶ Invited 10:20–10:40

Microsphere with Dimple Morphology Prepared from Ferulic Acid

Hironori ATARASHI

Okayama University

I112-13-I06 ▶ Invited 10:40–11:00

Thermally Conductive Hierarchical Molecular Assemblies Based on Filamentous Viruses

 Toshiki SAWADA^{1,2}
¹Tokyo Institute of Technology, ²PRESTO-JST

I112-13-I07 ▶ Invited 11:00–11:20

New Polyhydroxyalkanoate Biosynthesis Utilizing Metabolic Pathways for Amino Acid and Fatty Acid

Takeharu TSUGE

Tokyo Institute of Technology

December 13, 2019

Poster Session

Time 14:00–15:30 Room Trade-0

I1-13-P01

Characterization of Porous Ti6Al4V/Bio-based Polymer Composites for Improved Biocompatibility

 Mari MIYATA¹, Naritoshi AOYAGI¹, Kasumi FURUYA¹, Shota FUNAMI¹, Chuen Kum LEE²
¹National Institute of Technology, Nagaoka College,

²Nanyang Polytechnic, School of Engineering

I1-13-P02

Fabrication of Insulin-like Growth Factor-1 Conjugated IPN gel and Controlling Length of the Conjugation Linker for Enhancement of the Embedded Chondrocytes Function

 Hiro YAMAGUCHI¹, Shohei ISHIKAWA¹, Shigehito OSAWA^{1,2}, Michihiro IJIMA³, Hidenori OTSUKA^{1,2}
¹Graduate School of Science, Tokyo University of Science,

²Department of Applied Chemistry, Faculty of Science, Tokyo University of Science,

³Department of Materials Chemistry and Bioengineering, National Institute of Technology, Oyama College

December 12–13, 2019

Symposium I-2

Environmentally Degradable Polymers

[Organizers]

Jun KIKUCHI (RIKEN CSRS)

Sijun Dong (Institute of Urban Environment, Chinese Academy of Sciences)

December 12, 2019

Oral Session 5

Time 14:00–16:00 Room Mont-4

Chairperson Jun KIKUCHI

Opening Talk

Jun Kikuchi

14:00–14:00

I2-12-K01 ▶ Keynote 14:00–14:30

Recent advances in marine plastic pollution research in Japan

Atsuhiko ISOBE

Kyushu University

I2-12-I02 ▶ Invited 14:30–14:50

Study on the biological toxic effects of microplastics on *Oryzias melastigma*Sijun DONG, Xu ZHANG, Dongxiao DING, Yi LIN

Institute of Urban Environment, Chinese Academy of Sciences

I2-12-003 14:50–15:05

Measurement Informatics for Evaluation of Materials and Environment

Jun KIKUCHI

RIKEN CSRS

I2-12-I04 ▶ Invited 15:05–15:25

Molecular, Material, Product and Process Design and Process Control Based on Materials Informatics, Chemoinformatics and Process Informatics

Hiromasa KANEKO

Meiji University

I2-12-I05 ▶ Invited 15:25–15:45

Toward optimization of total environment: forward prediction and parameter optimization in MI

Kei TERAYAMA¹¹RIKEN Center for Advanced Intelligence Project, ²Medical Sciences Innovation Hub Program, RIKEN Cluster for Science, Technology and Innovation Hub, ³Department of Biomedical Data Intelligence, Graduate School of Medicine, Kyoto University

I2-12-I06 ▶ Invited 15:45–16:00

Quantum chemistry towards Fugaku

Takahito NAKAJIMA

RIKEN

December 12, 2019

Oral Session 6

Time 16:30–18:30 Room Mont-4

Chairperson Yoshifumi AMAMOTO

I2-12-I07 ▶ Invited 16:30–16:50

Silk-based materials as eco-friendly material

Keiji NUMATA

RIKEN

I2-12-I08 ▶ Invited 16:50–17:10

Biomass Plastics and Biodegradable Plastics - Solution of Circular Economy? -

Hiroshi SANO

Mitsubishi Chemical Corporation

I2-12-I09 ▶ Invited 17:10–17:30

Biodegradability of biodegradable plastics in marine environments

Ken-ichi KASUYA

Gunma University

I2-12-I10 ▶ Invited 17:30–17:50

Fermentative Production of PHBH and metabolic engineering for regulation of its material properties

Shunsuke SATO, Hisashi ARIKAWA, Yoshihiro MOURI, Sho FURUTATE

KANEKA CORPORATION

I2-12-I11 ▶ Invited 17:50–18:10

L₁ regularization and its application to polymerKei HIROSE¹, Keisuke TERAMOTO¹¹Kyushu University, ²RIKEN Center for Advanced Intelligence Project

I2-12-I12 ▶ Invited 18:10–18:30

Simulation and Informatics for Research of Polymer Materials

Ryuichi SAKASHITA

TOSOH

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I

December 13, 2019

Oral Session 7
Time 9:00–11:20 **Room** Mont-1

 Chairperson Hideki ABE, Takeharu TSUGE

I112-13-001 9:00–9:15

Development of Heat-resistant Polymeric Materials from Bio-based Chemicals
Hideki ABE

RIKEN Center for Sustainable Resource Science

I112-13-K02 ▶ Keynote 9:15–9:45

Controlled/Living Polymerization of Functional Styrenes from Natural Resources
Kotaro SATOH

Tokyo Institute of Technology

I112-13-003 9:45–10:00

Fabrication of Multiple Parallel Gel Filaments by Applying Shear to Polymer Assembly
Yuriko TAKAYAMA, Norihiro KATO

Utsunomiya University

I112-13-I04 ▶ Invited 10:00–10:20

Protease-catalyzed Polymerization for Synthesis of Polypeptides with Specific Sequence Motifs
Kousuke TSUCHIYA^{1,2}, Keiji NUMATA^{1,2}
¹RIKEN, ²JST-ERATO

I112-13-I05 ▶ Invited 10:20–10:40

Microsphere with Dimple Morphology Prepared from Ferulic Acid
Hironori ATARASHI

Okayama University

I112-13-I06 ▶ Invited 10:40–11:00

Thermally Conductive Hierarchical Molecular Assemblies Based on Filamentous Viruses
Toshiki SAWADA^{1,2}
¹Tokyo Institute of Technology, ²PRESTO-JST

I112-13-I07 ▶ Invited 11:00–11:20

New Polyhydroxyalkanoate Biosynthesis Utilizing Metabolic Pathways for Amino Acid and Fatty Acid
Takeharu TSUGE

Tokyo Institute of Technology

December 13, 2019

Poster Session
Time 14:00–15:30 **Room** Trade-0

I2-13-P01
Characterization of Scratch Damage of Commercial Polymers
Tomoko KAJIWARA¹, Yoshifumi AMAMOTO^{1,2}, Ken KOJIO^{1,2}, Atsushi TAKAHARA^{1,2}
¹Institute for Materials Chemistry and Engineering, Kyushu University, ²International Institute for Carbon-Neutral Energy Research, Kyushu University

I2-13-P02
Preparation and Characterization of Sacran/Imogolite Nanotubes Hybrid Film Prepared by Layer-by-Layer Assembly
Linlin LI¹, Wei MA², Akihiko TAKADA³, Yuji HIGAKI⁴, Maiko OKAJIMA⁵, Tatsuo KANEKO⁵, Atsushi TAKAHARA^{1,2,3}
¹Graduate School of Engineering, Kyushu University, ²International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, ³Institute for Materials Chemistry and Engineering (IMCE), Kyushu University, ⁴Department of Integrated Science and Technology, Faculty of Science and Technology, Oita University, ⁵School of Materials Science, Japan Advanced Institute of Science and Technology (JAIST)

I2-13-P03
Refining Messy NMR Data Important for Measurement Informatics
Shunji YAMADA^{1,2}, Atsushi KUROTANI², Eisuke CHIKAYAMA^{2,3}, Jun KIKUCHI^{1,2,4}
¹Nagoya University, ²RIKEN, ³Niigata University of International and Information Studies, ⁴Yokohama City University

I2-13-P04
Methods for Important Factor Extraction toward Membrane Interface Evaluation
Sosei SUZUKI

Graduate School of Medical Life Science, Yokohama City University

I2-13-P05
Analysis of Lignin Degradation by Fungi Isolated from West Coast, Sabah, Malaysia
Clarence M. ONGKUDON, Adznila EBERAHIM, Jun KIKUCHI, Abygail Lorna ERIC, Mailin MISSON, Minami MATSUI, Tomoko MATSUMOTO, Daiki YOKOYAMA

Universiti Malaysia Sabah

I2-13-P06**Synthesis of Oligopeptide Containing Natural and Unnatural Amino Acids Toward Environmentally Degradable Polymers**

Chie KOGANEMARU¹, Yoshifumi AMAMOTO^{1,2,3},
Atsushi TAKAHARA^{1,2,3}

¹Graduate School of Engineering, Kyushu University,
²Institute for Materials Chemistry and Engineering, Kyushu University,
³International Institute for Carbon-Neutral Energy Research, Kyushu University

I2-13-P07**Integrated Analysis of Biodegradable Plastics for Revealing the Relationship among Physical Properties and Chemical Structures**

Ryo YAMAWAKI¹, Yuuri TSUBOI², Akiyo TEI², Kengo ITO^{1,2},
Jun KIKUCHI^{1,2,3}

¹Grad. Sch. Med. Life Sci., Yokohama City Univ., ²RIKEN CSRS,
³Grad. Sch. Bioagri. Sci., Nagoya Univ.

I2-13-P08**Prediction of 2D J-resolved NMR parameters by combination of machine-learning and quantum chemical computations for molecular complexity**

Xiangru XU¹, Kengo ITO^{2,3}, Jun KIKUCHI^{2,3,4}

¹Institut des Sciences et Ingénierie Chimiques, Ecole Polytechnique Fédérale de Lausanne, ²RIKEN Center for Sustainable Resource Science, ³Graduate School of Medical Life Science, Yokohama City University, ⁴Graduate School of Bioagricultural Sciences, Nagoya University

December 12–14, 2019

Symposium I-3

Biodegradable Polymers for Biomedical Applications

[Organizer]

Masaya YAMAMOTO (Tohoku University)

December 12, 2019

Oral Session 6

Time 16:30–18:25 Room Mont-2

Chairpersons Yasuhiko IWASAKI, Tsuyoshi KIMURA

I3-12-I01 ▶ Invited 16:30–16:53

Development of cationic poly(amino acid)s for nucleic acids delivery

Kanjiro MIYATA

The University of Tokyo

I3-12-I02 ▶ Invited 16:53–17:16

Design of Soft-biomaterials Based on Intermediate Water Contents

Masaru TANAKA

Kyushu University

I3-12-I03 ▶ Invited 17:16–17:39

Temperature-Responsive Biodegradable Injectable Polymer Systems Exhibiting Irreversible Gelation for Medical Application

Yuichi OHYA

Kansai University

I3-12-I04 ▶ Invited 17:39–18:02

 Relationship of Structures and Biomedical Functions for Resorbable Poly(ϵ -caprolactone)-block-Poly(ethylene glycol) Copolymers

Ming-Fa HSIEH

Chung Yuan Christian University

I3-12-I05 ▶ Invited 18:02–18:25

Self-Assembling Elastin-Like Polypeptides as a Platform for Cell Studies

Ayae SUGAWARA-NARUTAKI

Nagoya University

December 13, 2019

Oral Session 7

Time 9:00–11:25 Room Mont-2

Chairpersons Shang-Hsiu HU, Nobuyuki MORIMOTO

I3-13-I01 ▶ Invited 9:00–9:23

Network formation of endothelial cells on decellularized ECM hydrogels

Tsuyoshi KIMURA¹, Janpei KADOTA¹, Naoko NAKAMURA², Yoshihide HASHIMOTO¹, Akio KISHIDA¹
¹Tokyo Medical and Dental University, ²Shibaura Institute of Technology

I3-13-I02 ▶ Invited 9:23–9:46

Increased Chemoresistance of Tumor Cells on Staged Tumorigenesis- Mimicking Matrices

Takashi HOSHIBA

Tokyo Metropolitan Industrial Technology Research Institute

I3-13-003 9:46–9:56

Preparation of stepwise osteogenesis-mimicking ECM-deposited PLGA-collagen hybrid meshes for tissue engineering

Yazhou CHEN^{1,2}, Naoki KAWAZOE¹, Guoping CHEN^{1,2}
¹Research Center for Functional Materials, National Institute for Materials Science, Tsukuba, 305-0044, Japan,

²Department of Materials Science and Engineering, Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba, 305-8577, Japan

I3-13-I04 ▶ Invited 9:56–10:19

Phosphorus-containing polymers for bone treatment

Yasuhiko IWASAKI

Kansai University

I3-13-I05 ▶ Invited 10:19–10:42

An Apoptotic Cell-inspired Polymer for Anti-inflammatory Therapy

Mitsuhiro EBARA

National Institute for Materials Science

I3-13-I06 ▶ Invited 10:42–11:05

A Fish Gelatin-based Soft Tissue Adhesive for Biomedical Applications

Tetsushi TAGUCHI

National Institute for Materials Science

I3-13-007

11:05–11:15

Deformation and formation of Lo phase domains on cell-sized Liposome with membrane-adhesive plasmonic nanomaterialsTomohiro NOBEYAMA¹, Shigyo KAZUKI², Hirotaka NAKATSUJI³, Hiroshi SUGIYAMA⁴, Tsutomu HAMADA⁵, Tatsuya MURAKAMI^{1,6}¹Graduate School of Engineering, Toyama Prefectural University, ²Bio-AFM Frontier Research Center, Kanazawa University, ³Graduate School of Engineering, Osaka University, ⁴Graduate School of Science, Kyoto University, ⁵School of Materials Science, Japan Advanced Institute Science and Technology, ⁶Institute for Integrated Cell-Material Sciences, Kyoto University

I3-13-008

11:15–11:25

Tunable non-enzymatic degradability of N-substituted polyaspartamide main chain for enhanced mRNA transfection efficiencyMitsuru NAITO¹, Yuta OTSU¹, Rimpei KAMEGAWA¹, Kotaro HAYASHI², Satoshi UCHIDA^{1,2}, Hyun Jin KIM¹, Kanjiro MIYATA¹¹The University of Tokyo, ²Innovation Center of NanoMedicine

December 13, 2019

Oral Session 8**Time** 14:00–15:52 **Room** Mont-2

Chairpersons Ming-Fa HSIEH, Mitsuhiro EBARA

I3-13-109 ▶ Invited

14:00–14:23

Polysaccharides-based Docking Hydrogels Bearing Biodegradable and Robust FunctionsTooru OOYA
Kobe University

I3-13-110 ▶ Invited

14:23–14:46

Adaptable Microporous Hydrogels for Neuron RegenerationShang-Hsiu HU
National Tsing Hua University

I3-13-111 ▶ Invited

14:46–15:09

Ultra-Flexible Nanofilms for Bio-Integrated Device & SystemToshinori FUJIE
Tokyo Institute of Technology

I3-13-112 ▶ Invited

15:09–15:32

Bioresorbable Inorganic/Organic Composite for Bone RepairMasanori KIKUCHI
National Institute for Materials Science

I3-13-013

15:32–15:42

Cell Separation Column using Temperature-Responsive-Cationic Copolymer Modified BeadsKenichi NAGASE¹, Daimu INANAGA¹, Goro EDATSUNE¹, Yuki NAGATA¹, Aya MIZUTANI AKIMOTO², Hideko KANAZAWA¹¹Keio University, ²The University of Tokyo

I3-13-014

15:42–15:52

Development of biomedical be-ta Ti alloys with low Young's modulus by selected laser melting from mixture powder

Mitsuharu TODAI

Department of Environmental Materials Engineering, National Institute of Technology, Niihama College

December 14, 2019

Oral Session 10**Time** 9:00–11:29 **Room** Work-3

Chairpersons Masaya YAMAMOTO, Jun-ichiro JO

I3-14-101 ▶ Invited

9:00–9:23

Biodegradable characteristics of octacalcium phosphate-based bone substitute materials involving osteoclastic cellular activityOsamu SUZUKI, Yukari SHIWAKU, Ryo HAMAI
Division of Craniofacial Function Engineering, Tohoku University Graduate School of Dentistry

I3-14-102 ▶ Invited

9:23–9:46

Development of Intracellular Controlled Release Technologies Based on Biodegradable Polymer Nanoparticles to Modify Cellular Biological ActivitiesJun-ichiro JO, Yasuhiko TABATA
Kyoto University

I3-14-103 ▶ Invited

9:46–10:09

Surface Modification of Silica Nanoparticles Using 4-Aryloxy Boron Dipyrromethene (BODIPY) Enhances Skin PermeationMasaru KATO
Showa University

I3-14-004

10:09–10:19

Reversible Stabilization of Messenger RNA-loaded Polyion Complex by Degradable Silica ShellRimpei KAMEGAWA¹, Mitsuru NAITO², Satoshi UCHIDA¹, Hyun Jin KIM², Kanjiro MIYATA¹¹Graduate School of Engineering, The University of Tokyo, ²Graduate School of Medicine, The University of Tokyo

I3-14-005

10:19–10:29

Design of sulfobetaine polymers for mitochondrial deliveryNobuyuki MORIMOTO, Yoshifumi OISHI, Masaya YAMAMOTO
Tohoku University

I3-14-006

10:29–10:39

Bifunctional scaffolds for photothermal breast cancer therapy and adipose tissue regeneration
Xiuhui WANG¹, Naoki KAWAZOE¹, Guoping CHEN^{1,2}
¹Research Center for Functional Materials, National Institute for Materials Science, ²Department of Materials Science and Engineering, Graduate School of Pure and Applied Sciences, University of Tsukuba

I3-14-007

10:39–10:49

Stimulation of Endogenous VEGF Secretion by Dodecyl group-modified Injectable Hydrogel
Yosuke MIZUNO¹, Tetsushi TAGUCHI^{1,2}
¹University of Tsukuba, ²National Institute for Materials Science

I3-14-008

10:49–10:59

New Cell Separation System using Mixed Temperature-responsive and Cationic Polymer Brushes
Haruno WAKAYAMA, Kenichi NAGASE, Hideko KANAZAWA
Keio University

I3-14-009

10:59–11:09

Regulation of Mesenchymal Stem Cells Transfection through Micropatterned Surfaces
Yongtao WANG¹, Yingjun YANG^{1,2}, Naoki KAWAZOE¹,
Guoping CHEN^{1,2}
¹National Institute of Materials for Science, ²University of Tsukuba

I3-14-010

11:09–11:19

Design of Cell Membrane Anchoring molecules for cell labeling
George MOGAMI
Tohoku University

I3-14-011

11:19–11:29

Magnetic Force-Assisted Sandwich Culture to Create 3D Microenvironment for Epithelial Cells
Masaya YAMAMOTO, Mayumi TOKUDA, Taiga SUTO
Tohoku University

Symposium A

Symposium B

Symposium C

Symposium D

Symposium E

Symposium F

Symposium G

Symposium H

Symposium I