

# The 10<sup>th</sup> Anniversary ACCMS-VO General Meeting

## Scientific Program

1<sup>st</sup> to 3<sup>rd</sup> November, 2015

Sakura Hall, Katahira-Campus, Tohoku University, Sendai, Japan

### *Time for*

*Keynote=30min talk+10min discussion*

*Invited=20min talk+5min discussion*

*Oral=15min talk+5min discussion*

**1<sup>st</sup> November, 2015 (Sunday)**

**Registration Desk Open from 8:30 to 18:00**

**Opening Remarks and a Special Talk (9:00 - 9:20)**

1. Greetings from the Director of IMRAM, Tohoku University

Atsushi Muramatsu

2. Special Talk

Yoshiyuki Kawazoe

“After several decades of period started computational materials research, now it is the time to make it reliable and useful from basic research to industrial applications”

**Session 1 (9:20 – 10:30) Organics and Carbon and Silicon-related Materials 1**

Chair: Kombiah Iyakutti

1. (Invited-1) “Detection of noncovalent bonding with dispersion-corrected first-principles calculations of Terahertz spectra”

Masae Takahashi

Graduate School of Agricultural Science, Tohoku University, Sendai, Japan

2. (Oral-1) “Study of Carbon crystals from nested K4 lattice to BC-8 structure”  
Katsumi Hagita, Ryoji Sahara, and Yoshiyuki Kawazoe  
Department of Applied Physics, National Defense Academy, Yokosuka, Japan
3. (Oral-2) “A giant Stark effect of functionalized Scandium carbides MXene: a first-principles study”  
Yunye Liang, Yoshiyuki Kawazoe, Ahmad Ranjbar, and Mohammad Khazaei  
New Industry Creation Hatchery Center, Tohoku University, Aobaku, Sendai, Japan

**Coffee Break (10:30 - 10:45)**

**Session 2 (10:45 - 12:35) New Physical Phenomena 1**

Chair: Kaito Takahashi

1. (Invited-2) “Superconductivity and metal-insulator transition in 5d iridium oxides”  
Seiji Yunoki  
RIKEN, Japan
2. (Oral-3) “Ultrafast electron-hole pair kinetics from linear response theory”  
Shota Ono  
Department of Physics, Graduate School of Engineering, Yokohama National University,  
Yokohama, Japan
3. (Oral-4) “Electronic switching in ReRAM devices”  
Hannes Raebiger, Antonio Claudio M. Padilha, Alexandre R. Rocha, and Gustavo M.  
Dalpian  
Department of Physics, Yokohama National University, Yokohama, Japan
4. (Oral-5) “The first-principles mapping onto the phase field crystal model”  
Swastibrata Bhattacharyya, Kaoru Ohno and Ryoji Sahara  
Department of Physics, Yokohama National University, Yokohama, Japan
5. (Oral-6) “Structure and Chemical Activity of Complex Modified Catalysts”  
Nurbosyn U. Zhanpeisov  
Institute for Excellence in Higher Education & Chemistry Department, Graduate School of  
Science, Tohoku University, Sendai, Japan

**12:35- 13:35 Lunch (buffet style)**

**Session 3 (13:35- 14:15) Keynote Talk 1**

Chair: Masae Takahashi

"Recent Progress in Theories of Thermal Transport"

Keivan Esfarjani

Department of Mechanical and Aerospace Engineering, Rutgers University, USA

**Session 4 (14:15-15:50) Materials Informatics Special Session 1**

Chair: Abhijit Chatterjee

1. (Oral-7) "Introductory speech - How to Evaluate and Certify the Reliability of Materials Data for Materials Informatics in Industrial Applications"

Yoshiyuki Kawazoe

New Industry Creation Hatchery Center, Tohoku University, Sendai, Japan

2. (Invited-3) "NIMS Materials Database and Knowledge Discovery"

Hidehiro Onodera, Masayoshi Yamazaki, and Masato Shimono

National Institute for Materials Science (NIMS), Tsukuba, Ibaraki, Japan

3. (Invited-4) "First-Principles Local-Energy and Local-Stress Analysis of Materials Interfaces"

Masanori Kohyama, Somesh Kr. Bhattacharya, Hao Wang, Vikas Sharma, Shingo Tanaka, and Yoshinori Shiihara

Research Institute of Electrochemical Energy, National Institute of Advanced Industrial Science and Technology (AIST), Ikeda, Osaka, Japan

4. (Oral-8) "Strategy to Accelerate Material R&D - Material Informatics & Multiscale Modeling"

Satoru Yamamoto

Dassault Systemes BIOVIA, ThinkPark Tower, Tokyo

**15:50 – 16:05 Coffee Break**

## **Session 5 (16:05 – 18:10) Materials Informatics Special Session 2**

Chairs: Yoshiyuki Kawazoe and Abhijit Chatterjee

1. (Invited-5) “Multidisciplinary Optimization of Epoxy Resin Based on Molecular Dynamics Simulation”  
Yutaka Oya, Tomonaga Okabe, Koichi Tanabe, and Gota Kikugawa  
Department of Aerospace Engineering, Tohoku University, Sendai, Japan
2. (Invited-6) “Three roles of materials information for material science”  
Kohmei Halada  
National Institute for Materials Science, Japan
3. (Invited-7) “Development of Simulation Open Platform for Materials Design”  
Minho Lee, Sangsoo Han, Seungchul Kim, Hiroshi Mizuseki, and Kwang-Ryeol Lee  
Computational Science Center, Korea Institute of Science and Technology, Seoul, Korea
4. (Invited-8) “Automation of first-principles calculations: why and how”  
KanghoonYim, Kyuhyun Lee, Joohee Lee, Yong Youn, and Seungwu Han  
Department of Materials Science and Engineering, Seoul National University, Seoul, Korea
5. (Oral-9) “Material informatics: the current state and the future vision from a software perspective”  
Abhijit Chatterjee  
Material Science Enterprise, Dassault Systemes Biovia, Tokyo, Japan

## **Poster Session with Food and Drink (18:10 - 20:10) – 24 Posters**

**2<sup>nd</sup> November, 2015 (Monday)**

## **Session 6 (9:00 - 10:15) Surfaces and Interfaces**

Chair: Jer-Lai Kuo

1. (Invited-9) “Development of Multi-Physics Simulators Based on Quantum Chemical Molecular Dynamics Method for Tribology, MEMS, and Energy Systems”  
Momoji Kubo

Institute for Materials Research, Tohoku University, Sendai, Japan

2. (Invited-10) “Metal-free catalysts: ORR, CO tolerance and oxidation and CO<sub>2</sub> hydrogenation”

Ranjit Thapa, S. Sinthika, and E. Mathan Kumar

SRM Research Institute, SRM University, Kattankulathur, Tamil Nadu, India

3. (Oral-10) “Effect of Oxidation Reaction on Low Friction Mechanism of Diamond-like Carbon in Water Lubrication: A Computational Study”

Shandan Bai, Jingxiang Xu, Yuji Higuchi, Nobuki Ozawa, Koshi Adachi, Shigeyuki Mori, Kazue Kurihara, and Momoji Kubo

New Industry Creation Hatchery Center, Tohoku University, Sendai, Japan

#### **Coffee Break (10:15 - 10:30)**

#### **Session 7 (10:30 – 12:05) Water Related Studies**

Chair: Sirichok Jungthawan

1. (Invited-11) “Structures and Dynamics of Supercool and Nano-confined Water from Empirical to *Ab-Initio* Molecular Dynamics”

Jer-Lai Kuo

Institute of Atomic and Molecular Science, Academia Sinica, Taipei, Taiwan

2. (Invited-12) “Competition between H<sub>2</sub>O and (H<sub>2</sub>O)<sub>2</sub> reaction with H<sub>2</sub>COO/CH<sub>3</sub>CHOO”

Kaito Takahashi, Liang-Chun Lin, and Jim Jr-Min Lin

Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan

3. (Oral-11) “Thermodynamics and Lattice Dynamics of Aragonite, Post-Aragonite and Shortite Crystals from Computer Simulations”

Talgat Inerbaev, Pavel Gavryushkin, and Konstantin Litasov

L.N. Gumilyov Eurasian National University, Astana, Kazakhstan

4. (Oral-12) “Anomaly of water viscosity behavior near the 273K”

Valery K. Malinovsky, Ravil K. Zhdanov, Kirill V. Gets, Vladimir R. Belosludov, Valerya A. Zykova, and Nikolay V. Surovtsev

Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

**12:05 - 13:20 Lunch (buffet style) and Group Photo**

**Session 8 (13:20 – 14:00) Keynote Talk 2**

Chair: Nurbosyn U. Zhanpeisov

"The Role of Clathrate Hydrates for Solving the Ecological and Energetical Problems"

Vladimir R. Belosludov

Nikolaev Institute of Inorganic Chemistry, Siberian Branch, Russian Academy of Sciences,  
Russia

**Session 9 (14:00-15:15) New Physical Phenomena 2**

Chair: Ying Chen

1. (Invited-13) "Axion electrodynamics description of magnetic ordering on edges of topological insulators"

Jisoon Ihm, Yea-Lee Lee, HeeChul Park, and Young-Woo Son

Department of Physics and Astronomy, Center for Theoretical Physics, Seoul National University, Seoul, Korea

2. (Invited-14) "Charge-induced Phase Transitions in Ferroelectric Superlattices"

Khian-Hooi Chew

Department of Physics, University of Malaya, Kuala Lumpur, Malaysia

3. (Oral-13) "Elastic properties of Fe-C and Fe-N martensites"

Maaouia Souissi, and Hiroshi Numakura

Department of Materials Science, Osaka Prefecture University, Sakai, Japan

**Coffee Break (15:15 - 15:30)**

**Session 10 (15:30 – 16:45) Clusters**

Chair: Rodion V. Belosludov

1. (Invited-15) "Reactions of NO on Copper Clusters Including Additive Metal Atom"

Shinichi Hirabayashi, and Masahiko Ichihashi

Cluster Research Laboratory, Toyota Technological Institute; in East Tokyo Laboratory,  
Genesis Research Institute, Inc., Chiba, Japan

2. (Invited-16) “Reaction Kinetics of CO Oxidation Catalyzed by Uni-Sized Pt Clusters Directly Bound to Si Surface”

Hisato Yasumatsu, and Nobuyuki Fukui

Cluster Research Laboratory, Toyota Technological Institute; in East Tokyo Laboratory,  
Genesis Research Institute, Inc., Chiba, Japan

3. (Oral-14) “Term rules for simple metal clusters: benchmark calculations of Al<sub>2</sub>, Al<sub>3</sub>, and Al<sub>4</sub>”

Daisuke Yoshida, and Hannes Raebiger

Department of Physics, Yokohama National University, Japan

### **Session 11 (16:45 - 18:40) Gas Storage**

Chair: Khian-Hooi Chew

1. (Invited-17) “Computational Design and Screening of Gas Separation Materials”

Hiroshi Mizuseki

Center for Computational Science, Korea Institute of Science and Technology, Seoul,  
Republic of Korea

2. (Invited-18) “Theoretical Study of Functional Nanoporous Materials”

Rodion Belosludov, and Yoshiyuki Kawazoe

Institute for Materials Research, Tohoku University, Sendai, Japan

3. (Oral-15) “The self-preservation effect of hydrates as applied to hydrogen storage”

Rodion V. Belosludov, Yulia Yu. Bozhko, Ravil K. Zhdanov, Oleg S. Subbotin, Vladimir R.  
Belosludov, and Yoshiyuki Kawazoe

Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

4. (Oral-16) “Development of Micro-Kinetic Mechanism for Water-Gas-Shift Reaction on Ni Surfaces”

Mingxia Zhou, Thong Le, Bin Liu, and Lam K. Huynh

International University, Vietnam National University at Ho Chi Minh City, Vietnam

5. (Oral-17) “Strategies to Improve Functionalized Silsesquioxane Frameworks for H<sub>2</sub> Storage”

Yun-Wen Chen, Amol Deshmukh, and Jer-Lai Kuo

Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan

### **19:00 - 21:00 Banquet with Sponsors Presentation**

#### **Celebration for the 10<sup>th</sup> Anniversary of ACCMS-VO**

Chair: Y. Kawazoe

1. ONR Global: Yoko Furukawa
2. Network Dynamics: Yuki Sakamoto
3. Bosch Japan: Masafumi Miyajima
4. Nihon-Technos: Ryuzo Aida
5. BIOVIA: Abhijit Chatterjee

#### **Poster Awards**

#### **VO-Electric Guitar Band**

Yoshiyuki Kawazoe, Kazuhiko Hongo, Kazuhiro Sato, Ryu Sakuma, Taiga Otaki

**3<sup>rd</sup> November, 2015 (Tuesday)**

### **Session 12 (9:00 - 10:35) Organics and Carbon and Silicon-related Materials 2**

Chair: Kwang-Ryeol Lee

1. (Invited-19) “Theoretical insights into the defect engineering process and minority carrier lifetime (MCL) in solar grade silicon solar cell”  
K. Iyakutti, Shinju, R. Rajeswarapalanichamy, V.J. Surya, and Y. Kawazoe  
Department of Physics and Nanotechnology, SRM University, Kattankulathur, Tamilnadu, India
2. (Invited-20) “Dirac Cone Move and Bandgap on/off Switching of Graphene Superlattice”  
Gang Chen and Yoshiyuki Kawazoe  
Laboratory of Advanced Materials Physics and Nanodevices, University of Jinan, P. R. China



3. (Oral-18) “Theoretical study of deformation behavior of strained porous graphene and its gas separation properties under pressure”

Sirichok Jungthawan, Yuwadee Suwan, and Sukit Limpijumnong

School of Physics, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima, Thailand

4. (Oral-19) “Theoretical Study on the o-Carborane Substituted Iridium Complexes for the Enhancement of Phosphorescence Efficiency”

Sang Uck Lee

Department of Applied Chemistry, Hanyang University, Ansan, Korea

### **Coffee Break (10:35 - 10:50)**

### **Session 13 (10:50 - 12:40) Crystals**

Chair: Keivan Esfarjani

1. (Invited-21) “Analysis of free energy calculation of the alloy system: Fe-Si as an example”

Ying Chen, Arkapol Saengdeejing, and Tetsuo Mohri

School of Engineering, Tohoku University, Japan

2. (Oral-20) “Momentum-dependent band spin splitting in MnO<sub>2</sub> crystals: A first-principles investigation”

Yusuke Noda, Kaoru Ohno, and Shinichiro Nakamura

RIKEN Innovation Center, Nakamura Laboratory, Saitama 351-0198, Japan

3. (Oral-21) “Structural and response properties of various phases of BaTiO<sub>3</sub> using different exchange correlation functionals and projector-augmented-wave potentials”

E. S. Goh, L. H. Ong, T. L. Yoon, and K. H. Chew

School of Physics, Universiti Sains Malaysia, Penang, Malaysia

4. (Oral-22) “Adsorption of Water Molecule on Beta-Form Belite Surface: Analysis Based on *Ab-Initio* Study”

Ryoji Sakurada, Masami Uzawa, Yoshifumi Hosokawa, Yoshiyuki Kawazoe, Aaditya Manjanath, and Abhishek Kumar Singh

Dept. of Civil Engineering, National Institute of Technology, Akita College, Japan

5. (Oral-23) “GGA and GGA+U modeling for atomic, electronic and magnetic structures of  $\text{Cr}_2\text{AlC}$ ”

Ahmad Ranjbar, and Seiji Yunoki

Computational Materials Science Research Team, RIKEN Advanced Institute for Computational Science, Kobe, Japan

### **12:40-13:40 Lunch (buffet style)**

### **Session 14 (13:40-14:20) Keynote Talk 3**

Chair: Masahiko Ichihashi

"Addressing the Challenges in Designing Efficient Thermoelectric Materials"

Abhishek Kumar Singh

Material Research Centre, Indian Institute of Science (IISc), India

### **Session 15 (14:20-16:20) TOMBO Version 2 Special Session**

Chair: Yoshiyuki Kawazoe

1. (Oral-24) “Introduction to TOMBO Approach”

Yoshiyuki Kawazoe

New Industry Creation Hatchery Center, Tohoku University, Sendai Japan

2. (Oral-25) “Case Study 1 with TOMBO: All Electron GW Calculations of Rutile  $\text{TiO}_2$  and  $\text{Ti}_{0.75}\text{Nb}_{0.25}\text{O}_2$ ”

Shota Ono

Yokohama National University, Yokohama, Japan

3. (Oral-26) “Case Study 2 with TOMBO: Self-Consistent Linearized  $\text{GW}\Gamma$  + Bethe-Salpeter Equation Approach for Small Atomic Systems”

Riichi Kuwahara

Dassault Systemes BIOVIA, ThinkPark Tower, Tokyo

4. (Invited -22) “TOMBO Version 2 Tutorial”

Kaoru Ohno

Yokohama National University, Yokohama, Japan

## Contents

- TOMBO Installation 5min
- Explanation of TOMBO Algorithm 10min
- Explanation of INPUT, COORDINATES files 10 min
- Example 1: Li<sub>2</sub> GW + BSE 5min
  - +How to Analyze Results 5min
- Example 2: Si LDA 5min
  - +How to Analyze Results 5min
- How to submit MD Jobs 5min

5. (Oral-27) “To increase usability of TOMBO: Introduction of Pipeline Pilot and TOMBO Interface” 20min

Riichi Kuwahara

Dassault Systemes BIOVIA, ThinkPark Tower, Tokyo

## **Closing Remarks (16:20-16:30)**

Yoshiyuki Kawazoe