

# The 12<sup>th</sup> (Last) ACCMS-VO General Meeting Scientific Program

17<sup>th</sup> to 19<sup>th</sup> December, 2017  
Sakura Hall, Tohoku University and Arkangel Geihinkan

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*Keynote Talk (25min., presentation + 5min., discussion)*

*Invited Talk (15 min., presentation + 5min., discussion)*

*Oral Talk (15 min., presentation + 5min., discussion)*  
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17<sup>th</sup> December, 2017 (Sunday)

9:00 - 18:00 Registration Desk Open

Session 1: Opening, Oxides (9:20 - 10:40)

Chair: Ryoji Sahara

9:20 - 9:40 (Greetings) “Greetings from the Director of IMRAM (Institute of Multidisciplinary Research for Advanced Materials), Tohoku University”

Atsushi Muramatsu

9:40 – 10:00 (Invited-1) “Design of transition-metal-doped TiO<sub>2</sub> as a multipurpose support for fuel cell application”

Meng-Che Tsai, John Rick, Wei-Nien Su and Bing-Joe Hwang

10:00 – 10:20 (Invited-2) “First-principles Calculation of Coefficient of Oxygen Self-diffusion in t-ZrO<sub>2</sub>”

Ying Chen, Hubin Luo, Lei Wang and Tetsuo Mohri

10:20 – 10:40 (Oral-1) “Oxygen migration and local structure change in ZrO<sub>2</sub> crystal with vacancies”

Yayoi Terada, Tetsuo Mohri

**10:40 - 11:10 Coffee Break**

**Session 2 (11:10 - 12:50) New Carbon Materials and MXenes**

Chair: Vladimir Belosludov

11:10 – 11:30 (Invited-3) “Computational prediction of new carbon allotropes in sp<sup>2</sup>-sp<sup>3</sup> bonding networks”

Jian-Tao Wang, Zhen-Zhen Li, Hiroshi Mizusek, and Yoshiyuki Kawazoe

11:30 – 11:50 (Oral-2) “Insight into exfoliation possibility of MAX phases into 2D MXenes”

Mohammad Khazaei and Seiji Yunoki

11:50 – 12:10 (Oral-3) “Magnetism in Cr-based MAX phases and their derivatives 2D MXenes”

Ahmad Ranjbar and Seiji Yunoki

12:10 – 12:30 (Oral-4) “Atomistic Origin of Phase Stability in Oxygen-Functionalized MXene”

Avanish Mishra, Pooja Srivastava, Abel Carreras, Isao Tanaka, Hiroshi Mizuseki, Kwang-Ryeol Lee, and Abhishek K. Singh

12:30 – 12:50 (Invited-4) “Spontaneous Ferroelectric Distortion Driven Weyl Semimetal in Oxide HgPbO<sub>3</sub>”

Ronghan Li, Yuanfeng Xu, Jianggang He, Sami Ullah, Jiangxiu Li, Jun-Ming Liu, Dianzhong Li, Cesare Franchini., Hongming Weng, and Xing-Qiu Chen

**12:50 - 14:00 Lunch (Buffet Style on the First Floor)**

**Session 3 (14:00 - 15:50) Keynote Talk-1, 2D Materials,**

Chair: Kaito Takahashi

14:00 – 14:30 (Keynote-1) “Theoretical Investigation on a New Two-dimensional Carbon Allotrope: Application in Optoelectronics and Photocatalysis”

Hiroshi Mizuseki

14:30 – 14:50 (Invited-5) “Recent Advances in Penta-Graphene: Heterojunctions Containing Penta-Graphene”

Qian Wang

14:50 – 15:10 (Invited-5) “Computational Material Design of Two Dimensional Materials and Their Energy Applications”

Jer-Lai Kuo

15:10 – 15:30 (Invited-7) “Flat Building Blocks for Flat Silicene”

Masae Takahashi

15:30 – 15:50 (Oral-5) “3D visualization by commodity virtual reality for computational material sciences”

Katsumi Hagita

**15:50 - 16:20 Coffee Break**

**Session 4 (16:20 - 17:40) Fullerenes**

Chair: Talgat Inerbaev

16:20 – 16:40 (invited-8) “Metal doped endohedral fullerene chains: thermoelectric properties”

V. R. Belosludov, R. K. Zhdanov, R.V. Belosludov, Y. Kawazoe

16:40 – 17:00 (Oral- 6) “Spectroscopic and theoretical studies on the structural, electronic, and optical properties of zinc octaethylporphyrin/C<sub>60</sub> co-deposited films for understanding the donor-acceptor interactions in organic solar cells”

J. Onoe, S. Watanabe, S. Kato, M. Nakaya, and J.-P. Bucher

17:00 – 17:20 (Oral-7) “Production of Li<sup>+</sup>@C<sub>60</sub>”

Kaoru Ohno, Aaditya Manjanath, and Yoshiyuki Kawazoe

17:20 – 17:40 (Oral-8) “Improvement of the thermoelectric properties of fullerene films by photo- and electron-beam-induced polymerization”

Masato Nakaya, Kentaro Yashiro, Shinta Watanabe, and Jun Onoe

**Poster Session with Food and Drink (17:40 - 20:00) - 30 posters -**

Chair: Rodion Beloslodov

**18<sup>th</sup> December, 2017 (Monday)**

**Session 5 (9:20 - 10:40) Reaction, Intermediate States, Experiments**

Chair: Qian Wang

9:20 – 9:40 (Invited-9) “VUV spectroscopy of fluoride crystals using various kinds of synchrotron radiations”

Nobuhiko Sarukura

9:40 – 10:00 (Invited-10) “How fast is the atmospheric photolysis rate of Criegee intermediates?”

Kangtao Yin and Kaito Takahashi

10:00 – 10:20 (Invited-11) “Reaction Dynamics of Mg(II)/Mg(I) Couple in a Water Cluster Toward Carbon Dioxide”

Chi-Kit (Andy) Siu

10:20 – 10:40 (Oral-9) “Atmospheric fate of Criegee Intermediates with up to three carbon atoms”

Cangtao Yin, Kaito Takahashi

**10:40 - 11:10 Coffee Break**

**Session 6 (11:10 - 12:50) : Clusters**

Chair: Khian-Hooi Chew

11:10 – 11:30 (Invited-12) “Activation of Methane on Metal Clusters”

Masahiko Ichihashi and Shinichi Hirabayashi

11:30 – 11:50 (Invited-13) “ “Low-temperature catalytic activity in CO oxidation and NO reduction by Pt clusters bound to Si surface having electron accumulation”

Hisato Yasumatsu and Nobuyuki Fukui

11:50 – 12:10 (Invited-14) “Theoretical DFT Study on Small Gold Nanocluster and Extended Au(111) Surface”

Nurbosyn U. Zhanpeisov

12:10 – 12:30 (Oral-10) “Molecular dynamics study for oxidation on Ti surface at elevated temperature”

Somesh Kr. Bhattacharya, Ryoji Sahara, Kyosuke Ueda, and Takayuki Narushima

12:30 – 12:50 (Oral-11) “Accurate Gaussian expansion method calculations using Jacobian coordinates for three-body Coulombic systems”

Takayuki Oyamada, Emiko Hiyama, Masanori Tachikawa

**12:50 - 13:00 Group Photo on the Sakura-Hall Stairs**

**13:00 - 14:00 Lunch (Buffet Style on the First Floor)**

**Session 7 (14:00 - 15:10) Keynote Talk-2, Energy, Biology, Medical Materials**

Chair: Jer-Lai Kuo

14:00 – 14:30 (Keynote-2) “Theoretical aspects in realization of functional nanomaterials for energy and medical applications”

Rodion Belosludov

14:30 – 14:50 (Invited-15) "Structural fluctuation of protein and water"

Fumio Hirata

14:50 – 15:10 (Oral-12) “ Ni nanoparticle-decorated graphene for non-enzymatic glucose sensing”

M. Souissi, S. Darvishi, F. Karimzadeh, M. Kharaziha, R. Sahara, S. Ahadian

## **Coffee Break (15:10 - 15:40)**

### **Session 8 (15:40 - 17:00) Topological Insulators**

Chair: Nurbosyn Zhanpeisov

15:40 – 16:00 (Invited-16) “Why Topology in Solids? : Intuitive Understanding of Topological Insulators and Weyl Semimetals”

Jisoon Ihm

16:00 – 16:20 (Invited-17) “Searching for Wider Gap Topological Insulator and Enhancing Charge-to-Spin Conversion”

Yuan Ping Feng

16:20 – 16:40 (Oral-13) “ Defect characterization in transition metal dichalcogenides by Raman spectroscopy”

Soungmin Bae, Hannes Raebiger, Ken-ichi Shudo

16:40 – 17:00 (Oral-14) ”Topological phases in transition metal dichalcogenides”

Mohammad Saeed Bahramy

**17:00 - 17:30 Move to the Arcangel Geihinkan, Sendai**

**17:30 - 20:30 Banquet with Award Ceremony, Sponsor Presentations, and Abdul Kalam Professor Position Party for Prof. Kawazoe**

Chair: Kaoru Ohno

1. The Best Poster Awards for ACCMS-VO12
2. The ACCMS Mid Career Award
3. Sponsor presentations
  1. ONR Global, ITC-PAC, AOARD

## 2. Sendai Tourism, Convention and International Association

### Music Played by the VO Electric Guitar Band

Yoshiyuki Kawazoe(G), Kazuhiko Hongo(D), Kazuhiro Sato(G), Miyuki Matsuda(K), and Taiga Otaki(B)

**19<sup>th</sup> December, 2017 (Tuesday)**

### **Session 9 (9:20 - 10:40) Battery and Energy Materials**

Chair: Masahiko Ichihashi

9:20 – 9:40 (Invited-18) “Theoretical Analysis on Li Ion Behavior near Li<sub>3</sub>PO<sub>4</sub>/Metal Interfaces and Its Response to Applied Voltages”

Satoshi Watanabe, Wei Liu, and Koji Shimizu

9:40 – 10:00 (Oral-15) “Dehydrogenation of MgH<sub>2</sub>: Layer dependent doping and screening based approach”

E. Mathan Kumar, A. Rajkamal and Ranjit Thapa

10:00 – 10:20 (Oral-16) “Sodiation Mechanism of Black Phosphorus/Graphite Heterostructures for Sodium Ion Batteries: A DFT approach”

Hong Woo Lee, Sang Soo Han

10:20 – 10:40 (Oral-17) “Atomistic Modeling and Simulation of M<sub>2</sub>B<sub>12</sub>H<sub>12</sub> (M = Li or Na)”

Kartik Sau, Tamio Ikeshoji, Shigeyuki Takagi, Shin-ichi Orimo

### **10:40 - 11:10 Coffee Break**

### **Session 10 (11:10 - 12:20) Materials Informatics, Multi-scale, New Method**

Chair: Hisato Yasumatsu

11:10 – 11:30 (Invited-19) “Supercomputer Post-K Project “Challenge of Basic Science - Exploring Extremes through Multi-Physics and Multi-Scale”

Momoji Kubo

11:30 – 11:50 (Invited-20) “Machine-Learning Assisted Accurate Band Gap Predictions of Functionalized MXene”

Arunkumar CR, Avanish Mishra, Rishabh Vaish, Swanti Satsangi, Hiroshi Mizuseki, Kwang-Ryeol Lee, and Abhishek K. Singh

11:50 – 12:10 (Invited-21) “Bayesian approach combined with first-principles simulations toward computational materials design”

Kenta Hongo

12:10 – 12:30 (Invited-22) “Probing Quantum Structures : How Theory complements Experiments”

G.P. Das

12:30 – 12:50 (Invited-23) “Energy relaxation in simple metals: Beyond the quasiequilibrium approach”

Shota Ono

**12:50 – 14:00 Lunch (Buffet Style on the First Floor)**

**Session 11 (14:00 - 15:20) Polymers, Magnetic Materials,**

Chair: Yin Chen

14:00 – 14:20 (Invited-24) “Structural change in polymer melt on increasing density studied by molecular dynamics simulation”

Yasuhiro Senda and Tomonori Kai

14:20 – 14:40 (Invited-25) “Stability of SmFe<sub>12</sub>-based Compounds: From Electronic Structure and Phonon Spectrum”

Arkapol Saengdeejing, Ying Chen

14:40 – 15:00 (Oral-18) “Spin torque effect in spin-filter based magnetic junctions”

Yu-Hui Tang



15:00 – 15:20 (Oral-19) “Spin Unrestricted Excited State Relaxation Dynamics in Semiconducting Systems”

Talgat Inerbaev and Dmitri S. Kilin

**Coffee Break (15:20 - 15:50)**

**Session 12 (15:50 - 17:30) Ferroelectrics, Structured Materials, Concluding Remarks**

Chair: Hiroshi Mizuseki

15:50 – 16:10 (Invited-26) “Correlation between Electronic, Polarization and Structural Properties of Domain Walls in BiFeO<sub>3</sub>”

Khian-Hooi Chew, Yun-Wen Chen, and Jer-Lai Kuo

16:10 – 16:30 (Invited-27) “ $\beta$ -CuGaO<sub>2</sub> as Strong Candidate Materials for Efficient Ferroelectric Photovoltaics”

Donghun Kim

16:30 – 16:50 (Oral-20) “Thermodynamic properties in Ni-Al system using a face-centered-cubic lattice model with a first-principles renormalized potential”

R. Sahara, T. Osada, S. Bhattacharyya, and K. Ohno

16:50 – 17:10 (Oral-21) “First-Principles Local-Energy and Local-Stress Calculations of Fe Grain Boundaries and Alloys”

Masanori Kohyama, Zhuo Xu, Somesh Kr. Bhattacharya, Shingo Tanaka, and Yoshinori Shiihara

17:10 – 17:30

(Closing Remarks) Yoshiyuki Kawazoe