

# The 11<sup>th</sup> ACCMS-VO General Meeting Scientific Program

19<sup>th</sup> to 21<sup>st</sup> December, 2016

Sakura Hall, Tohoku University and Arkangel Geihinkan

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

*Special Talk (25min. presentation + 5min. discussion)*

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

*Oral Talk (12 min. presentation + 3min. discussion)*  
-----

19<sup>th</sup> December, 2016 (Monday)

8:30 - 18:00 Registration Desk Open

Session 1 (9:00 - 10:40) Opening, Keynote Talk-1, Structures

Chair: Yoshiyuki Kawazoe

9:00-9:15 (Greetings) “Greetings from the Director of IMRAM (Institute of Multidisciplinary Research for Advanced Materials), Tohoku University”

Atsushi Muramatsu

9:15-9:45 (Keynote-1) “Spintronics with 2D materials - first principles explorations”

Yuan-Ping Feng<sup>1,2</sup>, Lei Shen<sup>3</sup>, Minggang Zeng<sup>4</sup>, Qingyun Wu<sup>5,1</sup>, Sandhya Chintalapati<sup>2,1</sup>

<sup>1</sup> *Department of Physics, National University of Singapore, Singapore*

<sup>2</sup> *Centre for Advanced 2D Materials, National University of Singapore, Singapore*

<sup>3</sup> *Engineering Science Programme, National University of Singapore, Singapore*

<sup>4</sup> *Data Storage Institute, A\*STAR, Singapore, Singapore*

<sup>5</sup> *Department of Materials Science and Engineering, National University of Singapore, Singapore*

9:45-10:05 (Invited-1) “Stability analysis of NdFe<sub>12</sub> series compounds as

promising new high performance permanent magnetic materials”

Ying Chen and Arkapol Saengdeejing

*School of Engineering, Tohoku University, 6-6-01 Aramakioba, Aoba-ku, Sendai, 980-8579, Japan*

10:05-10:25 (Invited-2) “Understanding of Abnormal Behaviors of S/PAN Composite Cathode in Lithium Sulfur Batteries”

Chen-Jui Huang<sup>a</sup>, Ju-Hsiang Cheng<sup>a</sup>, Ming-Hsien Lin<sup>a</sup>, Wei-Nien Su<sup>b</sup>, Pouya Partovi-Azar<sup>c</sup>, Payam Kaghazchi<sup>c,\*</sup>, and Bing-Joe Hwang<sup>a,d</sup>

<sup>a</sup> *NanoElectrochemistry Laboratory, Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei, 10607, Taiwan*

<sup>b</sup> *NanoElectrochemistry Laboratory, Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology, Taipei, 10607, Taiwan*

<sup>c</sup> *Institute for Physical and Theoretical Chemistry, Freie Universtaet, Berlin, Germany*

<sup>d</sup> *National Synchrotron Radiation Research Center, 30076, Hsin-Chu, Taiwan*

10:25-10:40 (Oral-1) “Dopants induced structural and electronic structure modification of TiO<sub>2</sub> particles”

Dai Quoc Ho<sup>1,2</sup>, Heechae Choi<sup>2,3</sup>, and Seungchul Kim<sup>1,2</sup>

<sup>1</sup> *Department of Nanomaterials Science and Engineering, Korea University of Science and Technology*

<sup>2</sup> *Computational Research Science Center, Korea Institute of Science and Technology*

<sup>3</sup> *Virtual Lab Inc.*

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

**Session 2 (11:10 - 12:35) Bulk Materials, Optical and Magnetic Properties**

Chair: Jer-Lai Kuo

11:10-11:30 (Invited-3) “High throughput design of efficient thermoelectric materials”

Abhishek Kumar Singh<sup>1, 2</sup> and Isao Tanaka<sup>2</sup>

<sup>1</sup> *Materials Research Centre, Indian Institute of Science, Bangalore 560012, India*

<sup>2</sup> *Department of Materials Science and Engineering, Kyoto University, Yoshida-Honmachi, Sakyo-ku, Kyoto 606-8501, Japan*

11:30-11:50 (Invited-4) "Bandgap narrowing of TiO<sub>2</sub> by co-doping"

Sutassana Na Phattalung,<sup>1</sup> Sukit Limpijumnong<sup>2</sup> and Jaejun Yu<sup>3</sup>

<sup>1</sup> *Department of Basic Science and Physical Education, Kasetsart University, Si Racha Campus 20230, Thailand*

<sup>2</sup> *School of Physics and NANOTEC-SUT Center of Excellence on Advanced Functional Nanomaterials, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand*

<sup>3</sup> *Center for Theoretical Physics, Department of Physics and Astronomy, Seoul National University, Seoul 08826, Republic of Korea*

11:50-12:05 (Oral-2) "Structural and Electronic Properties of BiFeO<sub>3</sub> Domain Walls"

Yun-Wen Chen<sup>1</sup>, Khian-Hooi Chew<sup>2</sup>, and Jer-Lai Kuo<sup>1</sup>

<sup>1</sup> *Department of Physics, University of Malaya, Malaysia*

<sup>2</sup> *Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan*

12:05-12:20 (Oral-3) "Spin Transport Calculation in Novel nm-scale Magnetic Junctions"

Yu-Hui Tang

*Department of Physics, National Central University, Zhong-Li, Taoyuan, Taiwan*

12:20-12:35 (Oral-4) "Optical properties of solar control materials studied by first-principles calculations"

Satoshi Yoshio<sup>1</sup>, Koichiro Maki<sup>1</sup>, Kenji Adachi<sup>2</sup>

<sup>1</sup> *Sumitomo Metal Mining Co., Ltd., Computer Aided Engineering and Development Dept., Tokyo, Japan*

<sup>2</sup> *Sumitomo Metal Mining Co., Ltd., Ichikawa Research Center, Ichikawa, Chiba, Japan*

**12:35 - 13:40 Lunch (Buffet Style) and Group Photo**

**Session 3 (13:40 - 15:45) Clusters and Nanoparticles, TOMBO Development**

Chair: Kaito Takahashi

13:40-14:00 (Invited-5) “Adsorption of CO<sub>2</sub> onto Copper-based Clusters”

Shinichi Hirabayashi<sup>1</sup> and Masahiko Ichihashi<sup>2</sup>

<sup>1</sup> *East Tokyo Laboratory, Genesis Research Institute, Inc., 717-86 Futamata, Ichikawa, Chiba 272-0001, Japan*

<sup>2</sup> *Cluster Research Laboratory, Toyota Technological Institute: in East Tokyo Laboratory, Genesis Research Institute, Inc., 717-86 Futamata, Ichikawa, Chiba 272-0001, Japan*

14:00-14:20(Invited-6) “Low-temperature and anti-CO-poisoning characteristics in catalytic CO oxidation driven by uni-sized Pt clusters directly bound to Si substrate, Pt<sub>N</sub>/Si”

Hisato Yasumatsu<sup>1</sup> and Nobuyuki Fukui<sup>2</sup>

<sup>1</sup> *Cluster Research Laboratory, Toyota Technological Institute:*

*In <sup>2</sup>East Tokyo Laboratory, Genesis Research Institute, 717-866 Futamata, Ichikawa, Chiba 272-0001, Japan*

14:20-14:40 (Invited-7) “First-principles Study on Graphene-based Materials for Heavy Metal Removal”

Hiroshi Mizuseki and Keunsu Choi

*Korea Institute of Science and Technology (KIST), Hwarangno 14-gil 5, Seongbuk-gu, Seoul 02792, Republic of Korea*

14:40-14:55 (Oral-5) “Electronic structures of MXenes and their possible applications”

Mohammad Khazaei and Seiji Yunoki

*RIKEN Advanced Institute for Computational Science, Kobe, Japan*

14:55-15:10 (Oral-6) “Structural, electronic and magnetic properties of Cr<sub>2</sub>AX (A= Al, Ge, Ga; and X= C, N, B) MAX phases”

Ahmad Ranjbar<sup>1</sup> and Seiji Yunoki<sup>1, 2, 3</sup>

<sup>1</sup> *Computational Materials Science Research Team, RIKEN Advanced Institute for Computational Science (AICS), Kobe, Hyogo 650-0047, Japan*

<sup>2</sup> *Computational Condensed Matter Physics Laboratory, RIKEN, Wako, Saitama 351-0198, Japan*

<sup>3</sup> *Computational Quantum Matter Research Team, RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama 351-0198, Japan*

15:10-15:25 (Oral-7) “Direct band gap fluoride under high pressure”

Nobuhiko Sarukura

*Institute of Laser Engineering, Osaka University, Osaka, Japan*

15:25-15:45 (Invited-8) “Recent Development of TOMBO Ver. 2”

Kaoru Ohno<sup>1</sup>, Riichi Kuwahara<sup>2</sup>, Yoshifumi Noguchi<sup>3</sup>, Nu Thi Pham<sup>1</sup>, Tomohiro Isobe<sup>1</sup>, Tsubasa Aoki<sup>1</sup>, Ryoji Sahara<sup>4</sup>, and Yoshiyuki Kawazoe<sup>5</sup>

<sup>1</sup> *Department of Physics, Yokohama National University, Yokohama 240-8501, Japan*

<sup>2</sup> *Dassault Systèmes BIOVIA K.K., ThinkPark Tower, Osaki, Tokyo 140-6020, Japan*

<sup>3</sup> *Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581, Japan*

<sup>4</sup> *National Institute for Materials Science, Sengen, Tsukuba 305-0047, Japan*

<sup>5</sup> *New Industry Creation Hatchery Center, Tohoku University, 980-8579 Japan*

**15:45 - 16:10 Coffee Break**

**Session 4 (16:10 - 17:45) Liquids, Ion Migration, Hydrogen Bond**

Chair: Talgat Inerbaev

16:10-16:30 (Invited-9) “Vibrational Signature of Proton in Hydrogen Bond Network: To Eigen or To Zundel”

Jer-Lai Kuo

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

16:30-16:50 (Invited-10) “Theoretical study on reactions of Criegee intermediates with water, hydrogen sulfide, ammonia, and methanol”

Kaito Takahashi

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

16:50-17:10 (Invited-11) “Study of extraction properties of ionic liquids with COSMO-RS”

M. Grabda<sup>1,2</sup>, M. Panigrahi<sup>1,3</sup>, D. Kozak<sup>1</sup>, E. Shibata<sup>1</sup>, T. Nakamura<sup>1</sup>

<sup>1</sup> *IMRAM, Tohoku University, Japan*

<sup>2</sup> *IEE PAS, Poland*

<sup>3</sup> *Bulent Ecevit University, Turkey*

17:10-17:25 (Oral-8) “Artificial Neural Network Modeling to Predict Viscosity of Oxide Glasses”

Jaekyun Hwang<sup>1</sup>, Yuta Tanaka<sup>2</sup>, Seiichiro Ishino<sup>3</sup>, Satoshi Watanabe<sup>1</sup>

<sup>1</sup> *Department of Materials Engineering, The University of Tokyo, Tokyo, Japan*

<sup>2</sup> *Department of Physics, The University of Tokyo, Tokyo, Japan*

<sup>3</sup> *Department of Applied Physics, The University of Tokyo, Tokyo, Japan*

17:25-17:45 (Invited-12) “Study of Ion Migration Behaviors in Novel Electronic Devices using Density Functional Calculations and Machine Learning”

Wenwen Li<sup>1</sup>, Yasunobu Ando<sup>2</sup>, E. Minamitani<sup>1</sup>, and Satoshi Watanabe<sup>1</sup>

<sup>1</sup> *Department of Materials Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*

<sup>2</sup> *Research Center for Computational Design of Advanced Functional Materials, National Institute of Advanced Industrial Science and Technology, 1-1-1 Umezono, Tsukuba, Ibaraki 305-8568, Japan*

**Poster Session with Food and Drink (17:45 - 20:00) - 25 posters -**

**20<sup>th</sup> December, 2016 (Tuesday)**

**Session 5 (9:00 - 10:40) Keynote Talk-2, Special Talk, Ice, Magnetic Property**

Chair: Rodion Belosludov

9:00-9:30 (Keynote-2) “Computational Materials Study for both Fundamental Science and Industrial Applications”

Jisoon Ihm

*Pohang University of Science and Technology, Korea*

9:30-9:50 (Invited-13) “The melting temperature of Ice”

John S. Tse

X. Yong,<sup>1</sup> C.J. Burnham,<sup>2</sup> N.J. English<sup>2</sup> and J.S. Tse<sup>1</sup>

<sup>1</sup> *Department of Physics and Engineering Physics, University of Saskatchewan, Saskatoon, SK S7N 0K4 Canada*

<sup>2</sup> *School of Chemical and Bioprocess Engineering, University College Dublin, Belfield, Dublin 4, Ireland.*

9:50-10:10 (Invited-14) “General Applications of the Pentagraphene Structure”

Katsumi Hagita<sup>1</sup> and Yoshiyuki Kawazoe<sup>2</sup>

<sup>1</sup> *National Defense Academy of Japan*

<sup>2</sup> *New Industry Creation Hatchery Center, Tohoku University*

10:10-10:40 (Special) "The Legacy of Walter Kohn"

Gour Prasad Das

*Indian Association for the Cultivation of Science (IACS), Kolkata-700032, INDIA*

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

**Session 6 (11:10 - 12:50) Special Session on Nanocarbon 1**

Chair: Yoshiyuki Kawazoe

11:10-11:20 (Greetings) “Materials R&D supported by Computational Science in NEDO Project”

Ken Kokubo

11:20-11:40 (Introduction) “NEDO Project: Computer-Aided Materials Design of

New Carbon Nanomaterials”

Kaoru Ohno

*Department of Physics, Yokohama National University, Yokohama 240-8501, Japan*

11:40-12:00 (Invited-15) “Simulation-Assisted Plasma Processing Power for Highly-Efficient Synthesis of Endohedral Fullerenes”

Rikizo Hatakeyama and Toshiro Kaneko

*Department of Electronic Engineering, Tohoku University, Sendai 980-8579, Japan*

12:00-12:20 (Invited-16) “Structure of Lithium-Cation Endohedral C<sub>60</sub> Fullerene and its Application to Energy Storage”

Eunsang Kwon,<sup>1</sup> Takeshi Matsukawa,<sup>2</sup> Akinori Hoshikawa,<sup>2</sup> Toru Ishigaki,<sup>2</sup> Haruhiko Ogasawara,<sup>3</sup> Kazuhiko Kawachi,<sup>4</sup> and Yasuhiko Kasama<sup>4</sup>

<sup>1</sup> *Research and Analytical Center for Giant Molecules, Graduate School of Science, Tohoku University, Sendai 980-8578, Japan*

<sup>2</sup> *Frontier Research Center for Applied Atomic Sciences, Ibaraki University, Ibaraki 319-1106, Japan*

<sup>3</sup> *Graduate School of Pharmaceutical Sciences, Tohoku University, Sendai 980-8578, Japan*

<sup>4</sup> *Idea International Co., Ltd. Sendai 980-8579, Japan*

12:20-12:35 (Oral-9) “Theoretical evaluation for the reactivity of activated fullerenes”

Naohiko Ikuma, Ken Kokubo, Takumi Oshima

*Division of Applied Chemistry, Graduate School of Engineering, Osaka University, Suita 565-0871, Japan*

12:35-12:50 (Oral-10) “Optical and Structural Properties of Endohedral Fullerene-Encapsulated Ion”

Yoshifumi Noguchi

*Institute for Solid State Physics, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, Japan*

**12:50 - 14:00 Lunch (Buffet Style)**

**Session 7 (14:00 - 15:40) Special Session on Nanocarbon 3**



Chair: Eunsang Kwon,

14:00-14:20 (Invited-17) “Radiochemical study of endohedral fullerenes and MD simulation”

Tsutomu Ohtsuki<sup>1</sup>, Kaoru Ohno<sup>2</sup>

<sup>1</sup> Research Reactor Institute, Kyoto University

<sup>2</sup> Department of Physics, Yokohama National University

(Invited-18) “Isomer- and size-selected photodissociation reactions of carbon cluster ions”

Fuminori Misaizu

*Department of Chemistry, Graduate School of Science, Tohoku University*

14:40-15:00 (Invited-19) “The role of the Jahn-Teller distortions of molecule C<sub>60</sub> in formation of covalent bond between molecules, polarons and self-trapped excited states in one-dimensional C<sub>60</sub> crystal”

Vladimir Belosludov<sup>1</sup>, R. V. Belosludov<sup>2</sup>, and Y.Kawazoe<sup>3</sup>

<sup>1</sup> *Nicolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia*

<sup>2</sup> *Institute for Material Research, Tohoku University, Sendai, Japan*

<sup>3</sup> *New Industry Hatchery Center, Tohoku University, Sendai, 980-8579, Japan*

15:00-15:20 (Invited-20) “Recent advances in penta-graphene-like two-dimensional materials”

Qian Wang

*Center for Applied Physics and Technology, College of Engineering, Peking University, Beijing 100871, China*

15:20-15:40 (Invited-21) “Electroconductive thin films prepared from Li<sup>+</sup>@C<sub>60</sub> PF<sub>6</sub><sup>-</sup> toluene solution on Au(111) substrates”

Mathias Wolf,<sup>1</sup> Izabela Rzeznicka,<sup>2</sup> Yutaka Shibata,<sup>3</sup> Shinji Kajimoto,<sup>3</sup> Yasuhiko Fujita,<sup>4</sup> and Hiroshi Fukumura<sup>3</sup>

<sup>1</sup> *Technical University Munich, Garching bei München, 85748 Germany*

<sup>2</sup> *Shibaura Institute of Technology, Saitama 337-8570, Japan*

<sup>3</sup> *Tohoku University, Sendai 980-8578 Japan*

<sup>4</sup> *Katholieke Universiteit Leuven, Leuven, 3000 Belgium*

## Coffee Break (15:40 - 16:10)

### Session 8 (16:10 - 17:55) Special Session on Nanocarbon 3

Chair: Kaoru Ohno

16:10-16:30 (Invited-22) “One-dimensional uneven-structured nanocarbon : Novel physical and chemical properties”

Jun Onoe

*Department of Materials, Physics, and Energy Engineering, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8603, Japan*

16:30-16:50 (Invited-23) “Theory of charge transfer exciton dissociation at the donor-acceptor interface: Combined impact of entropy and carrier delocalization”

Shota Ono<sup>1</sup> and Kaoru Ohno<sup>2</sup>

<sup>1</sup> *Department of Electrical, Electronic, and Computer Engineering, Gifu University, Gifu 501-1193, Japan*

<sup>2</sup> *Department of Physics, Yokohama National University, Yokohama 240-8501, Japan*

16:50-17:10 (Invited-24) “Topological Node-Line Semimetallic Behaviour in Three-Dimensional Morphed Graphene of BCO-C<sub>16</sub>”

Jian-Tao Wang,<sup>1</sup> Hongming Weng,<sup>1</sup> Zhong Fang,<sup>1</sup> and Yoshiyuki Kawazoe<sup>2</sup>

<sup>1</sup> *Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

<sup>2</sup> *New Industry Creation Hatchery Center, Tohoku University, Sendai 980-8579, Japan*

17:10-17:25 (Oral-11) “High density of states at the Fermi level in defective sp<sup>2</sup>-based nanocarbons”

Yusuke Noda<sup>1</sup>, Shota Ono<sup>2</sup>, and Kaoru Ohno<sup>3</sup>

<sup>1</sup> *“Materials research by Information Integration” Initiative (MI2I), National Institute for Materials Science (NIMS), Tsukuba, Ibaraki 305-0047, Japan*

<sup>2</sup> *Department of Electrical, Electronic, and Computer Engineering, Gifu University, Gifu 501-1193, Japan*

<sup>3</sup> *Department of Physics, Yokohama National University, Yokohama 240-8501, Japan*

17:25-17:40 (Oral-12) “Generalized Stone-Wales transformation in graphene by electron irradiation”

Aaditya Manjanath and Kaoru Ohno

*Department of Physics, Graduate School of Engineering, Yokohama National University, Yokohama, Japan*

17:40-17:55 (Oral-13) “Application of periodic sub-nanoscale space constructed from one-dimensional C<sub>60</sub> polymers and from C<sub>60</sub> molecules”

Masato Nakaya, Shinta Watanabe, and Jun Onoe

*Department of Physics, Materials and Energy Engineering, Nagoya University*

**17:55 - 18:30 Move to the Arcangel Geihinkan, Sendai**

**18:30 - 19:00 Interlude with Drinking at the Arcangel Geihinkan**

**19:00 - 21:00 Banquet with Award Ceremony, Sponsor Presentations, and 70<sup>th</sup> Anniversary Party of Prof. Kawazoe**

1. The Best Poster Awards for ACCMS-VO11
2. The ACCMS Mid Carrier Award
3. Sponsor presentations
  1. ONR Global, Yoko Furukawa
  2. NEDO, Ken Kokubo
  3. Sendai Tourism, Convention and International Association, Akihito Tanno
  4. TAIHEIYO CEMENT, Yoshifumi Hosokawa
  5. Network Dynamics, Hiroyuki Sakamoto
  6. Sangyo Times, Inc., Hideki Motai

Music Played by the VO Electric Guitar Band

Yoshiyuki Kawazoe(G), Kazuhiko Hongo(D), Kazuhiro Sato(G), Miyuki

Matsuda(K), and Taiga Otaki(B)

21<sup>st</sup> December, 2016 (Wednesday)

**Session 9 (9:00 - 10:35) Battery Materials, Energy Materials, Radiation**

Chair: Masahiko Ichihashi

9:00-9:20 (Invited-25) “First-Principles Simulations for Electrochemical Systems under the Bias: Evaluation of the Kinetic Parameters”

Tamio Ikeshoji

*National Institute of Advanced Industrial Science and Technology (AIST) and Technology Research Association Fuel Cell Cutting-Edge Research Center (FC-Cubic) Tohoku University*

9:20-9:40 (Invited-26) “Theoretical Evaluation of the Relationship between Carrier Mobility and Intermolecular Configurations in Organic Single Crystals”

Byeong Sun Jun<sup>1</sup> and Sang Uck Lee<sup>1,2</sup>

<sup>1</sup> *Department of Bionano Technology, Hanyang University, 55 Hanyangdaehak-ro, Sangnok-gu, Ansan 426-791 Korea*

<sup>2</sup> *Department of Applied Chemistry, Hanyang University, 55 Hanyangdaehak-ro, Sangnok-gu, Ansan 426-791 Korea*

(Invited-27) “Clathrate Hydrate for Energy Storage and Transport”

Rodion V. Belosludov<sup>1</sup>, R. K. Zhdanov<sup>2</sup>, Yu. Yu. Bozhko<sup>2</sup>, K. V. Gets<sup>2</sup>, O.S. Subbotin<sup>2</sup>, V. R. Belosludov<sup>2</sup>, and Y. Kawazoe<sup>3</sup>

<sup>1</sup> *Institute for Materials Research, Tohoku University, Sendai, 980-8577, Japan*

<sup>2</sup> *Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia*

<sup>3</sup> *New Industry Creation Hatchery Center, Tohoku University, Sendai, 980-8579*

10:00-10:15 (Oral-14) “Electrochemical stability of Li-ion-conducting solid electrolyte: a first-principles study with genetic algorithm and convex-hull procedure”

Yusuke Noda<sup>1</sup>, Koki Nakano<sup>2</sup>, Masanobu Nakayama<sup>1,2,3,4</sup>

<sup>1</sup>*“Materials research by Information Integration” Initiative (MI2I), National Institute for Materials Science (NIMS), Tsukuba, Ibaraki, Japan*

<sup>2</sup>*Department of Life Science and Applied Chemistry, Nagoya Institute of Technology, Nagoya, Aichi, Japan*

<sup>3</sup>*Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN), National Institute for Materials Science (NIMS), Tsukuba, Ibaraki, Japan*

<sup>4</sup>*Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, Kyoto, Japan*

10:15-10:35 (Invited-28) ”Phase diagram of irradiated materials from *ab-initio* assessment”

Duc Nguyen-Manh<sup>1</sup>, J.S. Wrobel<sup>1,2</sup>, M. Klimenkov<sup>3</sup>, S.L. Dudarev<sup>1</sup>

<sup>1</sup> *CCFE, Culham Science Centre, Abingdon, OX14 3DB, United Kingdom*

<sup>2</sup> *Warsaw University of Technology, Woloska 141, 02-811 Warsaw, Poland*

<sup>3</sup> *Karlsruhe Institute of Technology, Kaiserstra?e 12, 76131 Karlsruhe, Germany*

## 10:35 - 11:10 Coffee Break

## Session 10 (11:10 - 12:50) Materials Informatics, Thermal Properties

Chair: Hisato Yasumatsu

11:10-11:30 (Invited-29) “Path integral simulation on muoniated acetone radical”

Yuki Oba, Tsutomu Kawatsu, and Masanori Tachikawa

*Graduate School of NanoBioScience, Yokohama City University, Yokohama, Japan*

11:30-11:50 (Invited-30) “Efficient chemical compound search based on Bayesian inference”

Kenta Hongo<sup>1,2,3</sup>, Hisaki Ikebata<sup>4</sup>, Tetsu Isomura<sup>5</sup>, Ryo Maezono<sup>1</sup>, Ryo Yoshida<sup>2,4,6</sup>

<sup>1</sup> *School of Information Science, Japan Advanced Institute of Science and*

*Technology (JAIST), 1-1 Asahidai, Nomi, Ishikawa 923-1292, Japan,*

*<sup>2</sup> National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan,*

*<sup>3</sup> PRESTO, Japan Science and Technology Agency (JST), 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan,*

*<sup>4</sup> Department of Statistical Science, SOKENDAI, 10-3 Midori-cho, Tachikawa, Tokyo 190-8562, Japan,*

*<sup>5</sup> The KAITEKI Institute, Inc. Palace Building, 1-1 Marunouchi 1-chome, Chiyoda-ku, Tokyo 100-8251, Japan,*

*<sup>6</sup> The Institute of Statistical Mathematics (ISM), 10-3 Midori-cho, Tachikawa, Tokyo 190- 8562, Japan*

11:50-12:10 (Invited-31) “New Era of Computational Materials Science led by the Web Platforms and Cloud Computing”

Minho Lee<sup>1</sup>, Seung-Chul Kim<sup>2</sup> and Kwang-Ryeol Lee<sup>2</sup>

*<sup>1</sup> Virtual Lab. Co. Ltd, Seoul, Korea*

*<sup>2</sup> Computational Science Center, Korea Institute of Science and Technology (KIST), Seoul, Korea*

12:10-12:30 (Invited-32) “The origin of quartic anharmonicity and negative thermal expansion of cubic ScF<sub>3</sub> and other D<sub>0h</sub> structure materials”

Sirichok Jungthawan<sup>1, 2, 3</sup>, Tipaporn Patniboon<sup>1</sup>, and Sukit Limpijumnong<sup>1, 2, 3</sup>

*<sup>1</sup> School of Physics, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand*

*<sup>2</sup> NANOTEC-SUT Center of Excellence on Advanced Functional Nanomaterials, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand*

*<sup>3</sup> Thailand Center of Excellence in Physics (ThEP), Commission on Higher Education, Bangkok 10400, Thailand*

12:30-12:50 (Invited-33) “First-principles study on electronic structures and thermoelectric properties of Cs-Ge type-I clathrates”

K. Akai, K. Kishimoto, T. Koyanagi, and S. Yamamoto  
*FGSS, Yamaguchi Univ., Yamaguchi, Japan.*

12:45 – 13:50 Lunch (Buffet Style)

**Session 11 (13:50 - 15:45) Mechanical Properties, Precipitates, Ferroelectrics**

Chair: Tamio Ikeshoji

13:50-14:10 (Invited-34) “Emergence of massless Dirac quasiparticles in correlated hydrogenated graphene with broken sublattice symmetry”

Seiji Yunoki

*RIKEN Advanced Institute for Computational Science, Kobe, Japan*

14:10-14:30 (Invited-35) “Large-Scale Molecular Dynamics Simulations on Degradation and Fracture Processes”

Momoji Kubo

*Institute for Materials Research, Tohoku University, Sendai, Japan*

14:30-14:50 (Invited-36) “First-Principles Local-Energy and Local-Stress Calculations of Materials Interfaces and Alloys”

Masanori Kohyama<sup>1</sup>, Somesh Kr. Bhattacharya<sup>1,2,#</sup>, Hao Wang<sup>1,3</sup>, Shingo Tanaka<sup>1</sup>, and Yoshinori Shiihara<sup>4</sup>

<sup>1</sup> *Research Institute of Electrochemical Energy, National Institute of Advanced Industrial Science and Technology (AIST), Ikeda, Osaka, Japan*

<sup>2</sup> *Elements Strategy Initiative for Structural Materials (ESISM), Kyoto University, Kyoto, Japan*

<sup>3</sup> *School of Materials Science and Engineering, Shanghai University, Shanghai, China*

<sup>4</sup> *Toyota Technological Institute, Tenpaku-ku, Nagoya, Japan*

<sup>#</sup> *Present Address: National Institute for Materials Science, Tsukuba, Japan*

14:50-15:10 (Invited-37) “First principles study of electronic structures and stability in structural materials”

Ryoji Sahara

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

15:01-15:25 (Oral-15) “First-principles study of stability of  $\gamma$ -Cr<sub>23-x</sub>Fe<sub>x</sub>C<sub>6</sub> precipitates: The effect of metal site occupancy”

Maaouia Souissi<sup>1</sup>, Ryoji Sahara<sup>1</sup>, Marcel H.F. Sluiter<sup>2</sup>, Tetsuya Matsunaga<sup>1</sup>,

and Masaaki Tabuchi<sup>1</sup>

<sup>1</sup> *Computational Structural Materials Design group, Research Center for Structural Materials, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan.*

<sup>2</sup> *Department of Materials Science and Engineering, Delft University of Technology, Mekelweg 2, 2628 CD Delft, The Netherlands.*

15:25-15:45 (Invited-38) "Non-Ising-like 180 degree Ferroelectric Domain Walls in BiFeO<sub>3</sub>"

Khian-Hooi Chew<sup>1</sup>, Yun-Wen Chen<sup>2</sup>, and Jer-Lai Kuo<sup>2</sup>

<sup>1</sup> *Department of Physics, University of Malaya, 50603 Kuala Lumpur, Malaysia*

<sup>2</sup> *Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan*

## **Coffee Break (15:45 - 16:10)**

## **Session 12 (16:10 - 17:40) Defects, Devices, Surfaces, Path Integral, Radiation, Concluding Remarks**

Chair: Ryoji Sahara

16:10-16:30 (Invited-39) "Defect physics without defects, and resistive memories"

Hannes Raebiger<sup>1,2</sup>, A. C. M. Padilha<sup>2,3</sup>, A. R. Rocha<sup>4</sup>, and G. M. Dalpian<sup>2</sup>

<sup>1</sup> *Department of Physics, Yokohama National University, Yokohama, Japan,*

<sup>2</sup> *CCNH, Universidade Federal do ABC, Santo Andr  - SP, Brazil,*

<sup>3</sup> *Physics Department, University of York, York, UK,*

<sup>4</sup> *IFT, Universidade Estadual Paulista, S o Paulo - SP, Brazil*

16:30-16:45 (Oral-16) "Multi-scale simulation for atomic force microscopy"

Yasuhiro Senda<sup>1</sup>, Janne Blomqvist<sup>2</sup>, Risto Nieminen<sup>2</sup>

<sup>1</sup> *Department of Applied Science, Yamaguchi University, Yamaguchi, 755-8611, Japan*

<sup>2</sup> *COMP Centre of Excellence, Department of Applied Physics, Aalto University, Finland*



16:45-17:00 (Oral-17) “Internal alterations of TbPc<sub>2</sub> molecules upon surface adsorption”

Anis Amorane<sup>1,2</sup>, Mario Ruben<sup>1,2</sup>, Svetlana Klyatskaya<sup>2</sup>, Jean-Pierre Bucher<sup>1</sup>

<sup>1</sup> *Institute of material physics and chemistry of Strasbourg (IPCMS). CNRS-Unistra. Strasbourg, France*

<sup>2</sup> *Institute of Nanotechnology. Karlsruhe institute of technology (KIT). Karlsruhe, Germany.*

17:00-17:20 (Invited-40) “Spin Unrestricted Excited State Relaxation Dynamics in Semiconducting Systems”

Talgat M. Inerbaev<sup>1,2</sup>, Stephanie J. Jensen<sup>3</sup>, Dmitri S. Kilin<sup>3,4</sup>

<sup>1</sup> *L. N. Gumilyov Eurasian National University, Astana, Kazakhstan*

<sup>2</sup> *National University of Science and Technology “MISIS”, Moscow, 119049 Russian Federation*

<sup>3</sup> *University of South Dakota, Vermillion, South Dakota, United States*

<sup>4</sup> *North Dakota State University, Fargo, North Dakota, United States*

17:20-17:40 (Invited-41) “Development of the depth-profiling sensor of radioactive Cs in pond sediment. - A computational contribution to the recovery from Fukushima disaster -”

Hiroshi Ogawa<sup>1</sup>, Kimitaka Minami<sup>1</sup>, Tohru Kawamoto<sup>1</sup>, Ramon Kanai<sup>2</sup>, Kohei Ishikawa<sup>2</sup>, and Ryuichi Kamimura<sup>2</sup>

<sup>1</sup> *National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, 305-8568, Japan*

<sup>2</sup> *Tokyo Power Technology Ltd. (TPT), Chiba, 267-0056, Japan*

(Closing Remarks) Yoshiyuki Kawazoe