

# **The 9<sup>th</sup> ACCMS-VO General Meeting Scientific Program**

**20<sup>th</sup> to 22<sup>nd</sup> December, 2014**

**Okinawa Institute of Science and Technology, Graduate University (OIST) and  
Sunmarina Hotel**

**20<sup>th</sup> December, 2014 (Saturday)**

**Breakfast (7:00 - 8:15) in Sunmarina Hotel**

**Moving to OIST by Bus (starting time = 8:15)**

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

**Opening Remarks and a Special Talk (9:00 - 9:30)**

Y. Kawazoe

“50 years of DFT and its Applications from Molecules to Bulk Materials”

**Session 1 (9:30 – 10:10) Keynote Talk 1**

Chair: G. P. Das

“Theory and Computer Simulations for Discovery of Materials”

Umesh V Waghmare

Theoretical Sciences Unit, J Nehru Centre for Advanced Scientific Research, Jakkur  
PO, Bangalore 560 064 INDIA

**Session 2 (10:10 - 11:35) Gas Production and Storage Materials**

Chair: H. Mizuseki

1. (Invited) “Clathrate hydrates as medium for hydrogen storage and self-preservation phenomena”

V. R. Belosludov, Yu.Yu. Bozhko, R.K. Zhdanov, O. S. Subbotin, R.V. Belosludov,  
and Y. Kawazoe

Kutateladze Institute of Thermophysics, SB RAS, Novosibirsk, Russia

2. (Oral) “Diffusivity of small gas molecules through porous graphene”  
Sirichok Jungthawan, Pakpoom Reunchan, and Sukit Limpijumnong  
School of Physics and NANOTEC-SUT Center of Excellence on Advanced Functional Nanomaterials, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand
  
3. (Oral) “Theoretical Study on Gas Separation in MOF Structures”  
Rodion Belosludov and Y. Kawazoe  
Institute for Materials Research, Tohoku University, Sendai, 980-8577, Japan
  
4. (Oral) “Theoretical study on Hydrogen Production and Storage”  
Jyh-Chiang Jiang  
Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei, 106, Taiwan, R.O.C.
  
5. (Oral) “Hydrogen adsorption on carbon-based materials: Application in magnetism and energy storage”  
Ahmad Ranjbar  
Computational Materials Science Research Team, RIKEN Advanced Institute for Computational Science (AICS), Kobe, Hyogo 650-0047, Japan

**11:35 - 12:45 Lunch**

**Session 3 (12:45- 14:40) Nanomaterials**

Chair: T. Inerbaev

1. (Invited) “Photodissociation dynamics of ClOOCl at wavelength longer than 300 nm”  
Julien Fremont, Kaito Takahashi  
Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, 10617 Taiwan
  
2. (Invited) “Ferromagnetism in Mg-doped AlN Surfaces and Nanowires”  
Sandhya Chintalapati, Lei Shen, and Yuan Ping Feng  
Department of Physics, National University of Singapore, Singapore

3. (Invited) “The emerging new family of two dimensional nanosheets”  
G. P. Das  
Department of Materials Science, Indian Association for the Cultivation of Science,  
Jadavpur, Kolkata – 700032, INDIA
  
4. (Invited) “Strong Electronic Interactions in Simple Cubic Calcium under Pressure”  
Udomsilp Pinsook, Teerachote Pakornchote, Prutthipong Tsuppayakorn-aek, Thiti  
Bovornratanaraks, Sornthep Vannarat  
Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok  
10330, Thailand
  
5. (Oral) “Production of Multi-Element Clusters by Cluster-Cluster-Collisions”  
Hideho Odaka and Masahiko Ichihashi  
Cluster Research Laboratory, Toyota Technological Institute: in East  
Tokyo Laboratory, Genesis Research Institute, Inc., 717-86 Futamata, Ichikawa,  
Chiba 272-0001, Japan

**14:40 – 14:55 Coffee Break**

**Session 4 (14:55 – 16:45) Carbon-related Materials**

Chair: R. Sahara

1. (Invited) “Topological Node-Line Semimetal in Three Dimensional Graphene Networks”  
Hongming Weng, Yunye Liang, Qiunan Xu, Rui Yu, Zhong Fang, Xi Dai, and  
Yoshiyuki Kawazoe  
Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics,  
Chinese Academy of Sciences, Beijing 100190, China
  
2. (Invited) “Electronic and magnetic properties of antidot patterned graphene  
supperlattices”  
G. Chen, Y. Y. Liang, and Y. Kawazoe  
Department of Physics, University of Jinan, Jinan, Shandong 250022, P. R. China
  
3. (Oral) “Magnetic properties and quantum phase of boron-carbon nanostructures”

Jun Ni

Department of Physics and State Key Laboratory of Low-Dimensional Quantum Physics, Tsinghua University, Beijing 100084, People's Republic of China

4. (Oral) “Challenges of graphene towards applications”  
V. Nam Do, H. Anh Le, S. Ta Ho, D. Chien Nguyen and T. Le  
Advanced Institute for Science and Technology (AIST), Hanoi University of Science and Technology (HUST), No. 01 Dai Co Viet road, Hanoi, Vietnam
  
5. (Oral) “High CO<sub>2</sub> capture capacity in stable metal-doped graphene systems: a theoretical trend study”  
Sherif A. Tawfik, X. Y. Cui, S. P. Ringer, and C. Stampfl  
School of Physics, The University of Sydney, Sydney, New South Wales, 2006, Australia
  
6. (Oral) “Decorating Graphene with Aromatic Structures via Coordination Bonds with Metal Atoms: Density Functional Theory Investigations”  
Hung M. Le, Yoshiyuki Kawazoe, Duc Nguyen-Manh  
Faculty of Materials Science, University of Science, Vietnam National University, Ho Chi Minh City, Vietnam

**Session 5 (16:45 – 18:55) Crystal Properties and its Growth**

Chair: G. Chen

1. (Invited) “Toward Accurate Calculation of Electronic and Structural Properties of Materials from First Principles”  
Shinji Tsuneyuki  
Department of Physics, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan
  
2. (Invited) “Stable three-dimensional metallic carbon and boron nitride”  
Qian Wang  
Center for Applied Physics and Technology, Peking University, Beijing 100871, China

3. (Invited) “Electron Transport Characteristics of Low-dimensional Carbon Allotropes”  
Eunyoung Choi and Sang Uck Lee  
Department of Applied Chemistry, Hanyang University, Ansan, Korea 426-791
  
4. (Invited) “Optical Properties of Graphene Derivatives”  
Haibin Su  
Nanyang Technological University, Singapore
  
5. (Oral) “Modified Micro-Pulling Down Crystal Growth Method to Improve the Radial Distribution of Dopant”  
Zhong Zeng, Long Qiao, Yaping Liu, Yuui Yokota, Yoshi Kawazoe, Akira Yoshikawa  
Department of Engineering Mechanics, College of Aerospace Engineering, Chongqing University, Chongqing 400044, China
  
6. (Oral) “Robust interface states in two-dimensional photonic crystals”  
Xueqin Huang, Meng Xiao, Z. Q. Zhang and C. T. Chan  
Department of Physics and Institute for Advanced Study, Hong Kong University of Science and Technology, Hong Kong, China

**Poster Session with Food and Drink (19:00 - 21:00) - 34 posters -**

**21<sup>st</sup> December, 2014 (Sunday)**

**Breakfast (7:00 - 8:15) in Sunmarina Hotel**

**Moving to OIST by Bus (starting time = 8:15)**

**Session 6 (9:00 - 9:40) Keynote Talk 2**

Chair: B. J. Huang

“Three-dimensional Three-connected Carbene with 3,4,6-Fold Helical Chains in all-sp<sup>2</sup> Bonding Networks”

Jian-Tao Wang

Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

## Session 7 (9:40 - 12:10) Chemical Reactions

Chair: J. L. Kuo

1. (Invited) “Non-Equilibrium Charge Dynamics in Functionalized Semiconductor Nanostructures”  
T. Inerbaev, D. Kilin  
Physical and Technical Department, Gumilyov Eurasian National University,  
Mirzoyan str., 2, Astana, 010008, Kazakhstan
2. (Invited) “DFT Calculations on Catalysts for Hydrogen Evolution Reaction”  
Bing-Joe Hwang and Men-Che Tsai  
Nanoelectrochemistry Laboratory, Department of Chemical Engineering, National  
Taiwan University of Science and Technology, Taipei 106, Taiwan, R. O. C.
3. (Invited) “Strain induced tuning of electronic and thermoelectric properties of TMDs”  
Atanu Samanta, Tribhuwan Pandey, Swastibrata Bhattacharyya, and Abhishek K. Singh  
Materials Research Center, Indian Institute of Science, Bangalore 560012, India
4. (Oral) “First Principles Studies of Water Splitting Mechanism on GaN Surfaces”  
Yun-Wen Chen and Jer-Lai Kuo  
Institute of Atomic and Molecular Sciences, Academia Sinica, No. 1, Roosevelt Rd.,  
Sec. 4, Taipei, 10617, Taiwan
5. (Oral) ”Organic solar cells based on capped-carbon nanotubes:  
End-cap geometry dependence of the power-conversion efficiency”  
Shota Ono, Kousei Tanikawa, Riichi Kuwahara, and Kaoru Ohno  
Department of Physics, Graduate School of Engineering, Yokohama National Univ.,  
Yokohama 240-8501, Japan
6. (Oral) “Theoretical DFT Study on Structure and Chemical Activity of Complex Modified Structures”  
Nurbosyn U. Zhanpeisov  
Institute for Excellence in Higher Education, Tohoku University, Sendai, Japan

7. (Oral) “Size Dependent Catalytic CO Oxidation Driven by Sub-Nano Platinum Clusters Directly Bound to Silicon Substrate”

Hisato Yasumatsu and Nobuyuki Fukui

Cluster Research Laboratory, Toyota Technological Institute: In East Tokyo Laboratory, Genesis Research Institute, Inc. 717-86 Futamata, Ichikawa, Chiba 272-0001, Japan

8. (Oral) “Multi-Physics Simulations on Semiconductor Processes by Tight-Binding Quantum Chemical Molecular Dynamics Method”

Momoji Kubo

Fracture and Reliability Research Institute, Graduate School of Engineering, Tohoku University, 6-6-11-701 Aoba Aramaki, Aoba-ku, Sendai 980-8579, Japan

### **12:10 - 13:30 Lunch and Group Photo**

### **Session 8 (13:30 - 14:55) Defects, Surface, and Interface 1**

Chair: Q. Sun

1. (Invited) “Adaptive-boost molecular dynamics simulation of thermally activated motions of crystal imperfections”

Shigenobu Ogata, Akio Ishii, Jun-Ping Du

Graduate School of Engineering Science, Osaka University, Osaka 560-8531, Japan

2. (Oral) “Combined Density Function Theory and Photoluminescence Investigation into the Surface Modification of CdSe Quantum Dots and Ligands”

Hung-lung Chou

Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology, Taipei 106, Taiwan R.O.C.

3. (Oral) “Quantum Chemical Molecular Dynamics Simulations of Gallium Nitride Chemical Mechanical Polishing Processes”

Kentaro Kawaguchi, Yuji Higuchi, Nobuki Ozawa, Momoji Kubo

Fracture and Reliability Research Institute (FRRI), Graduate School of Engineering, Tohoku University, 6-6-11-703 Aoba, Aramaki, Aoba-ku, Sendai 980-8579, Japan

4. (Oral) “First-Principles Study of  $\text{Li}_{4+x}\text{Ti}_5\text{O}_{12}$  Surfaces and Phase Boundaries”  
Shingo Tanaka, Mitsunori Kitta, Tomoyuki Tamura, Tomoki Akita, Yasushi Maeda,  
and Masanori Kohyama  
Research Institute for Ubiquitous Energy Devices (UBIQEN), National Institute of  
Advanced Industrial Science and Technology (AIST), Osaka 563-8577, Japan
5. (Oral) “High activity and low CO poisoning using noble metal-free catalysts: first  
principles study”  
S. Sinthika, E. Mathan Kumar, K. Iyakutti, Ranjit Thapa  
SRM Research Institute, SRM University, Kattankulathur-603203, Tamil Nadu,  
India

**Coffee Break (14:55 - 15:10)**

**Session 9 (15:10 - 16:45) Defects, Surface, and Interface 2**

Chair: R. Belosludov

1. (Invited) “Ferromagnetism of Mn-Containing Monolayers”  
Qiang Sun  
Department of Materials Science and Engineering, Peking University, Beijing  
100871, China
2. (Invited) “Geometric and Electronic Structures of Mono- and Di-vacancies in  
Phosphorene”  
Ting Hu and Jinming Dong  
Group of Computational Condensed Matter Physics, National Laboratory of Solid  
State Microstructures and Department of Physics, Nanjing University, Nanjing  
210093, P. R. China
3. (Oral) “Prediction of the trends on native defect properties in few-layer  
phosphorene”  
Vei Wang, and Yoshiyuki Kawazoe  
Department of Applied Physics, Xi’an University of Technology, Xi’an 710054,  
China
4. (Oral) “Effect of Trace Impurity on the Crystal Structure of Beta-Form Belite”



Ryoji Sakurada, Masami Uzawa, Yoshifumi Hosokawa, Yoshiyuki Kawazoe, and  
Abhishek Kumar Singh  
Dept. of Civil Engineering, Akita National College of Technology, JAPAN

5. (Oral) “Spin spitting in centrosymmetric solids”

Mohammad Saeed Bahramy

Quantum - Phase Electronics Center and Department of Applied Physics, The  
University of Tokyo, Tokyo 113 - 8655, Japan

### **Session 10 (16:45 - 18:10) Theories**

Chair: Q. Wang

1. (Invited) “Multiscale Materials Design for Novel Physical and Chemical Properties  
of Energy-related Materials”

Hiroshi Mizuseki

Center for Computational Science, Korea Institute of Science and Technology  
(KIST), Hwarangno 14-gil 5, Seongbuk-gu, Seoul, 136-791, Republic of Korea

2. (Oral) “Multi-scale model of AFM using MD/continuum coupling method”

Yasuhiro Senda, Shuji Shimamura, Janne Blomqvist, Risto Nieminen

Department of Applied Science, Yamaguchi University, Yamaguchi, 755-8611,  
Japan

3. (Oral) “Modern *ab-initio* calculations based on Tomas-Fermi-Dirac theory with  
quantum, correlation and multi-shells corrections”

Sergey Seriy

Alekseev Nizhny Novgorod state technical university. Russia, 681013,  
Komsomolsk-on-Amur, Lenina 23-25

4. (Oral) “Real-Space Real-Time Calculations tuned for K-computer”

Yasunari. Zempo, Nobuhiko Akino, Masaya. Ishida, Eiji

Tomiyama, and Hideki Yamamoto

Computer and Information Sciences, Hosei University, 3-7-2 Kajino Koganei,  
Tokyo 184-8584, Japan

5. (Oral) “Atomistic Observation of the Lithiation and Delithiation Behaviors of

Silicon Nanowires using Reactive Molecular Dynamics Simulations”

hyun Jung, minho Lee, byung chul Yeo, kwang-ryeol Lee, and sang soo Han

Center for Computational Science, Korea Institute of Science and Technology (KIST), Hwarangno 14-gil 5, Seongbuk-gu, Seoul 136-791, Republic of Korea

**18:10 - 19:00 Move to Sunmarina Hotel by Bus**

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

**Celebration for the 50<sup>th</sup> Anniversary of DFT**

Chair: Y. Kawazoe

1. ONR Global: Yoko Furukawa
2. CHAM Japan: Zuwei Kong
3. Network Dynamics: Yuki Sakamoto

**22<sup>nd</sup> December, 2014 (Monday)**

**Breakfast (7:00 - 8:15) in Sunmarina Hotel**

**Moving to OIST by Bus (starting time = 8:15)**

**Session 11 (9:00 - 10:35) Bulk Materials 1**

Chair: Y. P. Feng

1. (Invited) ”Exceptionally Long-ranged Lattice Relaxation in Oxygen-deficient Ta<sub>2</sub>O<sub>5</sub>”

Yong Yang, O. Sugino, and Y. Kawazoe

Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei 230031, China

2. (Invited) “Theory of Charge Compensation Phenomena for Polarization Discontinuities in Ferroelectric Superlattices”

Khian-Hooi Chew

Department of Physics, University of Malaya, 50603 Kuala Lumpur, Malaysia

3. (Oral) “*Ab Initio* Local-Energy and Local-Stress Calculations in Materials”

Masanori Kohyama, Somesh Kr. Bhattacharya, Hao Wang, Vikas Sharma, Shingo Tanaka, and Yoshinori Shiihara  
UBIQEN, National Institute of Advanced Industrial Science and Technology, Osaka, Japan

4. (Oral) “First-principles derivation of nonlinear elastic constants of single crystals”

Hajime Kimizuka, Takahiro Nishino, and Shigenobu Ogata

Department of Mechanical Science and Bioengineering, Osaka University, Osaka 560-8531, Japan

5. (Oral) “The Accurate Computation of the Negative Curie Temperature of PbTe”

Yue Chen and C. A. Marianetti

Department of Mechanical Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong

#### **Session 12 (10:35 – 12:00) : Bulk Materials 2**

Chair: N. U. Zhanpeisov

1. (Invited) “WEB 2.0 Based Nano Materials Design Platform”

Min-Ho Lee, Seungchul Kim, Sang-Soo Han, Kwang-Ryeol Lee

Center for Computational Science, Institute of Multidisciplinary Convergence of Matter, KIST, 39-1 Hawolgok-dong, Seongbuk-gu, Seoul, Korea

2. (Oral) “Anomalous Hall effect in Co-based Heusler compounds: an *ab initio* theoretical study”

Jen-Chuan Tung and Guang-Yu Guo

Center for General Education, China Medical University, Taichung 40402, Taiwan

3. (Oral) “First principle study of interaction between solute Si and screw dislocation in Fe-Si alloy”

Masato Wakeda and Shigenobu Ogata

Osaka University, Machikaneyama, Toyonaka 560-8531, Japan

4. (Oral) “First principles study of electronic structures and stability in structural materials”

Ryoji Sahara

National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, JAPAN

5. (Oral) “Solvation mechanism of task specific ionic liquids in water: A combined investigation using classical molecular dynamics and density functional theory”

Surya V.J. Yuvaraj, Ravil Zhdanov, Rodion V. Belosludov, Vladimir R. Belosludov, Oleg S. Subbotin, Kiyoshi Kanie, Kenji Funaki, Atsushi Muramatsu, Takashi Nakamura, Hiroshi Mizuseki, and Yoshiyuki Kawazoe

Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai – 980-8577, Japan.

**Closing Remarks (12:00 – 12:10)**

Y. Kawazoe

**12:20 - 13:30 Bus Trip to Okinawa Churaumi Aquarium (with Lunch Box)**

**13:30 – 15:30 Okinawa Churaumi Aquarium**

**15:30 – 18:00 Bus to Naha City**