

# **The 8<sup>th</sup> ACCMS-VO General Meeting Scientific Program**

7<sup>th</sup> to 9<sup>th</sup> November, 2013

Sakura Hall, Tohoku University and Hotel Matsushima Taikanso

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K-n: Keynote (1 hour, presentation + discussion)

I-m: Invited (30 min., presentation + discussion)

O-l: Oral (20 min., presentation + discussion)  
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## **7<sup>th</sup> November, 2013 (Thursday)**

**8:30 - 18:00 Registration Desk**

**Session 1 with Opening (9:00 - 10:30)**

Chair: Y. Kawazoe

Opening Remarks: Y. Kawazoe

(Invited) Hongming Weng, Xi Dai, and Zhong Fang, “Transition-Metal Pentatelluride  $\text{ZrTe}_5$  and  $\text{HfTe}_5$ : a Paradigm for Large-gap Quantum Spin Hall Insulators”

(Invited) Yong Yang and Yoshiyuki Kawazoe, “ Characterization of zero-point vibration in one-component crystals”

(Oral) Mohammad Saeed Bahramy, “Zeeman-- - like spin splitting controlled by an electric field”

**10:30 - 11:00 Coffee Break**

**Session 2 (11:00 - 12:10) Gas Storage Materials**

Chair: T. Ikeshoji

(Invited) K. Iyakutti, R. Lavanya, V. Vasu, V.J. Surya and Y. Kawazoe, “Hydrogen Storage in Ni+MgH<sub>2</sub> and Ti+MgH<sub>2</sub> clusters - A First Principles Study”

(Oral) Yu. Yu. Bozhko, O.S. Subbotin, R.V. Belosludov, H. Mizuseki, Y. Kawazoe, V.R. Belosludov and V.M. Fomin, “Modeling Structure and structural Transitions of Neon Hydrate”

(Oral) Ravil Zhdanov, Oleg Subbotin, Vladimir Belosludov, Rodion Belosludov and Yoshiyuki Kawazoe, “Theoretical Modeling of the Phase Diagram of Hydrogen Clathrate Hydrate in Wide Pressure Range”

**12:10 - 13:10 Lunch (Box Lunch) and Group Photo**

**Session 3 (13:10 - 15:40) Keynote Talk 1 and Nanostructures**

Chair: G. P. Das

(Keynote 1) K. Hirao, “The K Computer and Advanced Institute for Computational Science”

(Oral) Hannes Raebiger, “Transition Metal Atoms in Insulators: Point Defects and Embedded Nanostructures”

(Oral) Hideki Masuda, Hidehiro Yasuda and Jun Onoe, “Structural Analysis of Electron-Beam-Irradiated C<sub>60</sub> Single Crystal Film Using Electron Diffraction”

(Oral) Tetsuichiro Hayakawa, Kazuhiro Egashira, Masashi Arakawa, Tomonori Ito, Shun Sarugaku, Kota Ando, and Akira Terasaki, “X-Ray Spectroscopy of Size-Selected Free Metal-Oxide Clusters for Oxidation-State Analysis”

(Invited) G. Chen and Y. Kawazoe, “Role of Transition Metal in Catalyzing H<sub>2</sub> Splitting”

**15:40 - 16:10 Coffee Break**

**Session 4 (16:10 - 18:50) Bulk Alloy Systems and Energy Materials**

Chair: G. Chen

(Invited) Tribhuwan Pandey, and Abhishek K. Singh, “Origin of enhanced thermoelectric properties of doped CrSi<sub>2</sub>”

(Oral) Ryoji Sahara, Satoshi Emura, Seiichiro Ii, Shigenori Ueda, and Koichi Tsuchiya, “Simulation of Electronic Structures and Stability of Body-centered Cubic Ti-Mo Alloys by Special Quasirandom Structures”

(Oral) Tetsuo Mohri, “First-principles Calculation for Stability Analysis of Fe-Ni System”

(Oral) Abhijit Chatterjee, “Material Genomics a Preview of Future for Material”

(Oral) Hisato Yasumatsu and Nobuyuki Fukui, “Catalytic Function Induced by Charge Accumulated at Sub-Nano Interface Between Platinum Cluster Disk and Silicon Substrate”

(Invited) Jeoung Eui Hong, Kwang Sun Ryu, and Sang Uck Lee, “Electrochemical Characteristics of Halogen-doping Li<sub>4</sub>Ti<sub>5</sub>O<sub>12</sub> as Anode for Lithium-ion Batteries”

(Oral) Nurbosyn U. Zhanpeisov, “Theoretical DFT Study on Energy Materials and Some Insights on the Origin of Raman Band Shifts”

**Poster Session with Food and Drink (18:50 - 20:50) - 31 posters -**

1. Hiroki Kanehira, Muhammad Zainurin and Shuji Shimamura, “Theoretical Consideration of Fractoluminescence in Silicate Glass”

2. A.S. Trifonov, R.B. Vasiliev, I.S. Ezubchenko, M.S. Sokolikova, D.R. Britov, D.E. Presnov, O.V. Snigirev, R. Belosludov and H. Nejo “Mapping of Electronic Properties of Tetrapod-shaped Nanocrystals of CdTe/CdSe”
3. D.E. Presnov, V.V. Shorokhov, S.V. Amitonov, A.S. Trifonov, V.A. Krupenin, “Single Arsenic Atom SOI-based Single-electron Transistor”
4. H.Nejo, Y.Ogasawara and A.S.Trifonov, “A Mathematical Structure Appearing by Controlling Individual Molecules by Applying an Oscillating Voltage”
5. Hiroshi Ogawa, “Molecular Dynamics Study on the Structure and Kinetics of Dislocations in Vanadium Hydrides”
6. Keita Seto, Sen Zhang, James Koga, Hideo Nagatomo and Kunioki Mima, “Radiation Reaction via Quantum Vacuum”
7. Arkapol Saengdeejing, Ying Chen, Masashi Matsuura and Satoshi Sugimoto, “Electronic Structures and Formation Mechanism of Nd-O in Nd-Fe-B Magnets”
8. Takayuki Oyamada and Masanori Tachikawa, “Role of Electron-positron Correlation in Positron Attachment to LiH”
9. Shota Ono and Kaoru Ohno, “Acceleration of Three-dimensional Fourier Transformation to Obtain One-dimensional Radial Potential in TOMBO”
10. Shota Ono, Riichi Kuwahara and Kaoru Ohno, “Charge Separation Mechanism in a Complex System of Single-walled Carbon Nanotube and Zinc Phthalocyanine”
11. Nobuyuki Fukui and Hisato Yasumatsu, “Thermal Stability and Morphology of Pt Cluster Disk on Si(111) Surface”
12. Atsushi Suzuki and Takeo Oku, “Electronic Structure and Magnetic

Properties of Endohedral Metallofullerene Dimer of  $\text{Sc}_x\text{Y}_{3-x}\text{N}@\text{C}_{80}(\text{CF}_3)_n$  based on Mixed-Metal Nitride Cluster Fullerene”

13. Takeo Oku, Atsushi Suzuki and Tsuyoshi Akiyama, “Fabrication, Nanostructures and Photovoltaic Properties of Organic Thin Film Solar Cells with Inverted Structures”
14. Konstantin V. Vshivkov, “Particle-in-cell Simulation of Plasma Flow Acceleration in a Magnetic Channel”
15. Yusuke Noda, Keivan Esfarjani and Kaoru Ohno, “Thermoelectric Properties of Capped One-dimensional Peanut-shaped Fullerene Polymers”
16. V. J. Y. Surya, Y. Sivalingam, Y. Kawazoe, C. Di Natale and R. Paolesse, “DFT Study on Detection of Cysteine on Metalloporphyrins Coated ZnO Nanostructures”
17. Ming Zhang, Shota Ono and Kaoru Ohno, “GW Calculation of Electronic Structure of Titanium Dioxide with Nb Doping using TOMBO”
18. Hiroki Matsubara, Fabio Pichierri and Kazue Kurihara, “Molecular Dynamics Simulation on Nanoconfined Liquids”
19. K. Akai, K. Kishimoto, Y. Kono, S. Yamamoto and S. Shimamura, “Study of Alloy Effects for Electronic Structure on Sn-base Clathrates”
20. Kosuke Nakamura, Yuji Higuchi, Nobuki Ozawa, and Momoji Kubo, “Chemical Reaction Study between Cathode and Organic Solvent in Lithium-Ion Battery by Quantum Chemical Molecular Dynamics Method”
21. Yoshihiko Kobayashi, Seiichiro Sato, Shandan Bai, Yuji Higuchi, Nobuki Ozawa, Koshi Adachi, and Momoji Kubo, “Quantum Chemical Study on Chemical Reactions at Silicon Carbide Surface under Water Lubrication”

22. Shandan Bai, Yoshihiko Kobayashi, Seiichiro Sato, Yuji Higuchi, Nobuki Ozawa, Koshi Adachi, Jean Michel Martin, and Momoji Kubo, “Computational Simulation on Structure Change of Diamond-Like Carbon by Si Doping”
23. Yunye Liang and Yoshiyuki Kawazoe, “Half-Metallicity Modulation of hybrid BN-C nanotubes by external electric fields: A First-Principles Study.”
24. R. V. Belosludov, Y. Yokoyama, and D. V. Louzguine-Luzgin, “Theoretical Study on Zr-Cu-Al Metallic Glasses”
25. Nobuki Ozawa, Miho Nakamura, Kentaro Kawaguchi, Yuji Higuchi, and Momoji Kubo, “First-Principles Study on CMP Process of Glass Surface by Perovskite Oxide Abrasive Grain”
26. L. J. Kang, K. Akagi, and M.W. Chen, “First principles investigation of Lithium-air battery”
27. Keunsu Choi, Jaehyun Bae and Jisoon Ihm, “Investigation of insulating substrate for Silicene”
28. Heechae Choi, Kwang-Ryeol Lee, Sohye Cho and Seungchul Kim, “Formations of Intrinsic Point Defects of Bi-doped Y<sub>2</sub>O<sub>3</sub> and Their Effects in Photoluminescence”
29. K. Shida and Y. Kawazoe, “Approximated MCMC of Heisenberg-model with reduced usage of FFT”
30. Jian Zhou and Jinming Dong, “Band gap tuning in carbon doped silicene from first-principles calculations”
31. Katsumi Hagita, “Stress-strain relation of K4 Phenolic resins by classical MD simulation”

**8<sup>th</sup> November, 2013 (Friday)**

**Session 5 (9:00 - 10:30) Keynote Talk 2 and TOMBO Development**

Chair: R. Belosludov

(Keynote 2) K. Ohno, “Development of the all-electron mixed basis program, TOMBO”

(Invited) V. R. Belosludov, O. S. Subbotin, R. V. Belosludov, H. Mizuseki and Y. Kawazoe, “Formalism for Calculation Van der Waals Dispersion Coefficients within the All-electron Mixed-basis Approach”

**10:30 - 11:00 Coffee Break**

**Session 6 (11:00 - 12:00) : TOMBO Tutorial**

Chair: Y. Kawazoe

**12:00 - 13:00 Lunch (Box Lunch) and Poster Awarding Ceremony**

**Session 7 (13:00 - 15:00) Surface and Interface**

Chair: J. L. Kuo

(Invited) Chia-Ching Wang, Jyun-Yi Wu, and Jyh-Chiang Jiang, “Ammonia Oxidation on RuO<sub>2</sub>(110) Surfaces”

(Invited) T. M. Inerbaev, A. T. Akilbekov and A. K. Dauletbekova, “Water Interaction with Fluorine-Doped Co<sub>3</sub>O<sub>4</sub> (100) and (111) Surfaces”

(Oral) K.-H. Chew, K.-G. Lim, L.-H. Ong and M. Iwata, “Effect of Electrostatic Coupling and Interface Intermixing on Internal Electric Field and Polarization in Ferroelectric Superlattices”

(Oral) Sirichok Jungthawan and Worawat Meevasana, “First-principles Study of Potassium Intercalation in Hexagonal Molybdenum Disulfide (2H-MoS<sub>2</sub>)”

(Oral) Tamio Ikeshoji, “Ion Transfer in Solid and Polymer Electrolyte”

**Coffee Break (15:00 - 15:30)**

**Session 8 (15:30 - 17:00) Experimental and Basic Theories**

Chair: K. Ohno

(Invited) B. N. Dev, “Evolution of electronic structure and transport properties of ultra-thin films near the 2-D limit”

(Oral) Sergey Seriy, “Multi-fractal Basis for Wave-functions Approximation in *ab-initio* Calculations”

(Oral) Yoshihito Ogasawara, Shin’ichi Oishi, “On the Methods of Recognizing Natural Phenomena”

(Oral) Yayoi Terada, “Pressure Dependence of Phase Diagram on Polydisperse Lennard-Jones System”

**17:20 - 18:20 Move to Matsushima by Bus**

**19:00 - 21:00 Banquet**

**9<sup>th</sup> November, 2013 (Saturday)**

**Breakfast (7:00 - 9:00) in Hotel Matsushima Taikanso**

**Session 9 (9:00 - 10:20) Carbon-related Materials**

Chair: K. Iyakutti

(Invited) Jer-Lai Kuo, “2D Materials: Graphene, BN, TMD and Beyond”

(Invited) G.P. Das, C. Majumder, A.H.M. Abdul Wasey, and S. Chakrabarty,



“How to make inert h-BN monolayer catalytically active by providing transition metal support ?”

(Oral) Y. Y. Liang, Makoto Tagami, Hisashi Naito, Yoshiyuki Kawazoe, and Motoko Kotani, “All Carbon Mackay-like crystals with 8-fold symmetry”

**10:20 - 10:50 Coffee Break**

**Session 10 (10:50 - 12:00) : Chemical Reactions**

Chair: N. U. Zhanpeisov

(Invited) Hsueh-Chien Li, Jer-Lai Kuo, and Ming-Kang Tsai, “CO<sub>2</sub> Binding by Nucleophilic Attack: from Methodology Comparison to the Reaction Dynamics”

(Oral) Masahiko Ichihashi and Shinichi Hirabayashi, “Reactions of NO Molecules on Copper and Copper Oxide Cluster Ions”

(Oral) Momoji Kubo, “Tight-Binding Quantum Chemical Molecular Dynamics Simulations for Clarification of Chemical Mechanical Polishing Mechanism”

**Closing Remarks (12:00 - 12:30)**

**Y. Kawazoe**

**12:30 - 13:30 Lunch (Restraunt Shiosai)**

**14:00 - 16:30 Boat Trip in the Matsushima Bay + Godaido Tour**

**Move Back to Sendai by Bus (16:30 - 17:30)**