

**The 20<sup>th</sup> Anniversary of TOMBO and Russian Megagrant  
Opening International Conference**

- **With the Cerebration of Chongqing University Honorary Professorship  
Given to Prof. Kawazoe -**

21<sup>st</sup> and 22<sup>nd</sup> August, 2013

Newly Opened Katahira Seminar Room Espace, Tohoku University  
and the Westin Hotel Sendai

**SCIENTIFIC PROGRAM**

**21<sup>st</sup> August, 2013 (Wednesday)**

12:30 - 13:20 Registration

**Session 1: Chair: Y. Kawazoe**

13:20 - 13:30 Opening Y. Kawazoe, Tohoku University

13:30 - 14:00 H. Mizuseki, Korea Institute of Science and Technology,  
“Computational Materials Science by using the New Supercomputer in IMR  
- 27 Years with Prof. Kawazoe” (Keynote)

14:00 - 14:30 R. Belosludov, O. S. Subbotin, H. Mizuseki, V. R. Belosludov,  
and Y. Kawazoe, Tohoku University, “Description of properties of gas  
hydrates using interaction potentials evaluated from TOMBO program”  
(Invited)

14:30 - 15:00 S. Velappa, Tohoku University, "Some studies on pristine and  
functionalized graphene using first principles calculations"

15:00 - 15:30 Coffee Break

**Session 2: Chair: G. Chen**

15:30 - 16:00 J. T. Wang, C. F. Chen, and Y. Kawazoe, Chinese Academy of  
Sciences, "Kinetic Origin of Phase Transformation Pathways in Carbon,  
Silicon and Germanium" (Invited)

16:00 - 16:30 Z. Zeng, H. Mei, Z. Qiu, H. Mizuseki, and Y. Kawazoe, Chongqing University, "Numerical simulation of ACRT with a Fourier Legendre spectral element method" (Invited)

16:30 - 17:00 S. S. Han, Korea Institute of Science and Technology, "Improved Design of Metal Organic Frameworks for Efficient Gas Adsorption by Multi-scale Simulations" (Invited)

18:00-20:30 BANQUET

Westin Hotel Sendai

with Greeting from **the President of Tohoku University, Susumu Satomi**

**22<sup>nd</sup> August, 2013 (Thursday)**

**Session 3: Chair: Y. Kawazoe**

9:30 - 9:45 Opening: M. Kohyama, and T. Mohri

9:45 - 10:45 TOMBO tutorial: K. Ohno, R. Sahara, and Y. Kawazoe

10:45 - 11:15 Y. Noguchi, Tokyo University, "Optical properties of M+@C60 (M = H, Li, Na, and K): All-electron GW+Bethe-Salpeter method"

11:15 - 11:30 S. Ono, and K. Ohno, Yokohama National University, "Efficient electronic structure calculation in the mixed basis approach"

11:30 - 12:00 K. Ohno, R. Kuwahara, S. Ono, and M. Zhang, Yokohama National University, "Recent implementations of spectroscopy calculations in the all-electron mixed basis code, TOMBO" (Invited)

12:00 - 13:00 Lunch

**Session 4: Chair: Z. Nurobosyn**

13:00 - 13:30 M. S. Bahrany, RIKEN, Emergent phenomena in giant bulk Rashba semiconductors

13:30 - 14:00 V. R. Belosludov, O. S. Subbotin, R.V. Belosludov, H. Mizuseki, Y. Kawazoe, Siberian Branch-Russian Academy of Sciences, "Van der Waals interaction within density-functional theory in the all-electron mixed-basis TOMBO approach" (Invited)

14:00 - 14:30 Y. Y. Liang and Y. Kawazoe, Tohoku University, "Introduction of Wannier function into TOMBO"

14:30 - 15:00 R. Sahara, H. Mizuseki, M. H. F. Sluiter, K. Ohno, and Y. Kawazoe, National Institute for Materials Science, "Effect of a nickel cluster on the dissociation dynamics of a hydrogen molecule" (Invited)

15:00 - 15:30 Coffee Break

**Session 5: Chair: K. Ohno**

15:30 - 16:00 X. Hu, National Institute for Materials Science, "Novel Topological State in Perovskite Materials"(Invited)

16:00 - 16:30 Y. Chen, A. Saengdeejing and T. Mohri, Tohoku University, "Mechanomagneto effects in Fe-Si system" (Invited)

16:30 - 17:00 Y. Kawazoe, Tohoku University, "Present and Future of Our Collaboration"