1st RSC－CMSI Joint Seminar

**Strategic Crossover between High-Energy Photon Science and Computational Science for Multiscale Structure Science**

【Date】13:00～16:50, 15th (Sat.) Sep. 2012

【Venue】2F Conference Hall, SACLA Experimental Facility, RIKEN Harima Institute

【Language】Japanese

【Host】RIKEN SPring-8 Center (RSC)

&

Computational Materials Science Initiative (CMSI)

(Field 2 "New Materials and Energy Creation" within the Next-Generation Supercomputer Strategy Program of MEXT)

【Purpose】

The Synchrotron Radiation (SR) as a probe of electrons in materials can be considered a probe of materials function since the SR allows us to visualize the electrons distribution which governs the function. So far the electrons distribution mapping and electrostatic potential imaging using SPring-8 has visualized the function in crystals to develop structure science. On the other hand, an X-ray free electron laser 'SACLA' has a huge potential for changing the conventional structure-properties relationship research. The coherent X-ray of SACLA will be a promising tool to open the door to multiscale structure science in non-crystals such as polymers and phase-change materials. In order to visualize the function in the multiscale structure, the strategic use among SPring-8/SACLA/K computer is essential for us.

As the starting point, we have organized the first RSC-CMSI joint seminar 'Strategic Crossover between High-Energy Photon Science and Computational Science for Multiscale Structure Science'. In the present seminar, the experimental and computational scientists who develop the crossover use between the SR and High-Performance Computing (HPC) will give a talk in the viewpoint of multiscale structure science. We would like to discuss the organic use and collaboration among SPring-8/SACLA/K computer

【Program】

Chair: Kenichi Kato (RSC)

13:00～13:05
Opening Address: Director of RSC, Tetsuya Ishikawa

13:05～13:15
Masaki Takata (RSC)
“Perspective on Multiscale Structure Science”

13:15～13:40
Shinji Tsuneyuki (CMSI, The Univ. of Tokyo)
“Present Status and Future of Computational Materials Science by the Large-Scale Computing”

13:40～14:05
Shinji Kohara (JASRI/SPring-8)
“Visualization in the Nano-Scale Phase Change Mechanism by the Combination of the Reverse Monte Carlo Simulation and DFT calculation”

14:05～14:30
Eiji Nishibori (Nagoya Univ.)
Visualization of Materials Structure and Function by the Application of the Genetic Algorithm/MEM to Crystals

14:30～14:50　Coffee Break

Chair: Takashi Miyake (CMSI, AIST)

14:50～15:15
Hiroyuki Kishimoto (Sumitomo Rubber Industries, Ltd.)
“Design and Development of the Energy Saving Tire using Large-Scale Simulation based on the USAXS data”

15:15～15:40
Yuki Norizoe (JST/ERATO)
“Monte Carlo Simulation of 2-Dimensional Micro Structures of Polymer Brushes”

15:40～16:05
Yasumasa Joti (JASRI/XFEL)
“Bio-Supermolecule Imaging by the Crossover Use between SACLA and HPC”

16:05～16:45
Hidetoshi Fukuyama (Tokyo Univ. of Science)
“Contribution of Large-Scale Research Facilities to Problem Solving Science”

16:45～16:50
Closing Address: Deputy Director of RSC, Masaki Takata

17:00～17:50
SACLA Tour

18:00～19:30
Party (SPring-8 Special Cafeteria, Fee: 3,000 yen)

Organizers: K. Kato (RSC), M. Takata (RSC)
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