

Workshop on Advanced Structural Study

Date: 19th November, 2016.

Room B118, Natural Sciences Building B, University of Tsukuba

Co-hosts: International Education and Research Laboratory Program, University of Tsukuba

Tsukuba Research Center for Interdisciplinary Materials Science (TIMS)

Center for Integrated Research in Fundamental Science and Engineering (CiRfSE),

9:00- 9:10 Opening. Eiji Nishibori, University of Tsukuba.

Session 1: Accurate Structural Studies on Materials Science

9:15 -9:45 Hidetaka Kasai, University of Tsukuba & Aarhus University.

"Charge density study of layered metal dichalcogenides."

9:45 -10:15 Florian Kleemiss, Universität Bremen, Germany.

"Crystal and enzyme environmental effects on the electron density of a cysteine protease inhibitor."

10:15 -10:45 Eiji Nishibori & Venkatesha Rama Hathwar, University of Tsukuba

"Structural Studies at Structural Materials Sciences Lab of University of Tsukuba."

Break

Session 2: Advanced Experimental and Analytical Technique.

11:00 -11:30 Lorraine Andrade Malaspina, Universität Bremen, Germany.

"Hirshfeld Atom Refinement"

11:30 -12:00 Shinobu Aoyagi, Nagoya City University, Japan.

"Time-resolved structure analysis of resonantly vibrating quartz crystal"

12:30 -13:00 Bo Iversen, Aarhus University & University of Tsukuba,

"Accurate crystallography: densities, excited states and beyond crystals"

Lunch

Session 3: Award session and Radiation Damage.

14:00 -14:30 Yoshiki Kubota, Osaka Prefecture University, Japan.

Winner of The CRSJ Award 2016.

14:30 -15:00 Simon Grabowsky, Universität Bremen, Germany.

"Metal-organic compounds at synchrotrons. Can we overcome radiation damage?"

15:00 -15:30 Jacob Overgaard, Aarhus University, Denmark

"Charge densities and slow magnetization dynamics in a linear Fe(II) compound"

Break

Session 4: World Leading SR and Neutron Facilities in Japan.

15:45 -16:15 Takashi Ohara, J-PARC/JAERI

"Single crystal neutron diffraction experiments at J-PARC"

16:15 -16:45 Kuniyoshi Sugimoto, SPring-8/JASRI.

"Investigation of charge density study with CdTe pixel detector"

16:45 -17:30 Open discussion. Discussion Leader, Jacob Overgaard

17:30 -17:40 Closing. Bo Iversen.

