



The 1st Workshop of Reaction Infography (*R-ing*) Unit

11th June, 2019

Noyori Materials Science Laboratory, 2F Lecture Room

The World Research Unit (B-1) at Nagoya University “Reaction Infography (*R-ing*)” has been started since April 2019. The *R-ing* unit aims to prepare the new concept of reaction infography by collaborative researches on reaction imaging, informatics, and materials science. In this workshop, the concept of reaction infography and the frontiers of reaction imaging, materials informatics, and materials science are discussed.

Program

Session 1: Reaction Infography from the *R-ing* unit

- 10:00-10:30 Opening Remarks
Reaction Infography for Materials Science
Mizuki Tada (Nagoya Univ.)
- 10:30-11:00 Molecular Recognition and Trapping in the Nanospace of Metal-Organic Frameworks
Ryotaro Matsuda (Nagoya Univ.)
- 11:00-11:30 Laser Reaction Microscope: Real-time Imaging of Ultrafast Chemistry
Akiyoshi Hishikawa (Nagoya Univ.)
- 11:30-12:00 Looking for the Bridge between Photo-organic Synthesis and Surface Catalysis Science
Susumu Saito (Nagoya Univ.)

【Photo · Lunch】

Session 2: Frontiers of Materials Science

- 13:00-13:30 XAS- and DFT-based Mechanistic Study on Iron Catalysis in Organic Chemistry
Hikaru Takaya (Kyoto Univ.)
- 13:30-14:00 *Operando* Electrochemistry of Coordination Polymers: Discovery of New Species and Mechanism
Zhongyue Zhang (Nagoya Univ.)
- 14:00-14:30 Investigation of the Origin of Reaction Distribution in All-solid-state Lithium Ion Battery Cathode by Using CT-XAFS
Yuta Kimura (Tohoku Univ.)
- 14:30-15:00 Finding New Polymorphs of Layered Transition Metal Dichalcogenides
Shintaro Ishiwata (Osaka Univ.)

Session 3: Methodology of Reaction Imaging and Informatics for Materials Science

- 15:30-16:00 Tracking Chemical Reactions in Solution with Ultrashort X-ray Pulses
Shin-ichi Adachi (KEK)
- 16:00-16:30 Soft X-ray Core-level Spectroscopy Measurements for Catalytic Surface Reactions
Hiroshi Kondoh (Keio Univ.)
- 16:30-17:00 Knowledge Discovery from Materials Data
Dam Hieu Chi (JAIST)
- 17:00-17:30 Machine Learning and DFT Simulation for XAFS/EELS
Teruyasu Mizoguchi (Univ. Tokyo)
- 17:30-17:40 Concluding Remarks
Kunio Awaga (Nagoya Univ.)
- 18:00~ Banquet @ Hanano-ki