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 — Mizuki Tada (Nagoya Univ)

Reaction Infography for Materials Science

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 Ishiwatari (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