

# The 3rd Workshop of the Reaction Infography (R-ing) Unit

10-11, December, 2020 Virtual Symposium on ZOOM

The visualization of chemical reactions and functions is essential to understand functional materials. "Reaction Infography" is a term defined to visualize the key factors of chemical reactions and functions of materials and understand the black box of functionality. The R-ing Unit has been started since 2019 as the collaborative unit with the fields of visualization, informatics, and materials science to create a new master concept of material science based on Reaction Infography. In this workshop, we invite frontier researchers on visualization and material sciences and discuss the progress and development of reaction infography.

## Program

### Day 1

**Session 1: Invited Lectures** (Chair: Susumu Saito/ Co-Chair: Yuki Harada)

- 13:00-13:15 Opening Remarks: Introduction of Reaction Infography  
Mizuki Tada (Nagoya Univ.)
- 13:15-13:45 Molecular Dynamics Simulation of Nucleation Process in Binary Lennard-Jones System  
Satoshi Watanabe (Kyoto Univ.)
- 13:45-14:15 Lattice Strain-Driven Pathway Selection in Multicomponent Self-Assembly  
Hiroshi Sato (Univ. Tokyo.)
- 14:15-14:35 Dynamic Photochemical Reactions in the Flexible Nanoporous Metal Complexes  
Shinpei Kusaka (Nagoya Univ.)
- 14:35-14:55 Topology Derived Quantum Spin Liquid State in a 2D Metal-Organic Framework  
Zhongyue Zhang (Nagoya Univ.)

【Break 15 min】

**Session 2: Invited Lectures** (Chair: Mizuki Tada/ Co-Chair: Akira Yonezu)

- 15:10-15:40 Catalytic Surface Reactions Studied by Operando Soft X-ray Spectroscopy  
Susumu Yamamoto (Tohoku Univ.)
- 15:40-16:10 Advanced Many Electron Wave Function Theory and Computations for Photochemical Reactions  
Takeshi Yanai (Nagoya Univ.)
- 16:10-16:40 Structures and Reactions of Adsorbed Molecules Studied by High-resolution Scanning Probe Microscopy  
Tomoko Shimizu (Keio Univ.)
- 16:40-17:10 Next Generation Operando Soft X-ray Spectroscopy to Visualize Impact of Water on Material Functions  
Yoshihisa Harada (Univ. Tokyo)

【Break 15 min】

**Session 3: Plenary Lecture** (Chair: Ryotaro Matsuda)

- 17:25-18:10 Solving Reaction Infography Challenges by the next generation Synchrotron Radiation Facility  
Masaki Takata (Tohoku Univ.)

## Day 2

### *Session 4: Plenary Lecture* (Chair: Akiyoshi Hishikawa)

09:00-09:45 New Generation High Power Laser Systems Based on Multidimensional Dynamics in Hollow Core Fiber

François Légaré (INRS)

### *Session 5: Invited Lectures* (Chair: Xiaoguang Wang and Toshinobu Nakajo)

9:45-10:15 Strong-field Ionization, Rescattering, and Target Structure Imaging with Vortex Electrons

Toru Morishita (Univ. E-Commun.)

**【Break 10 min】**

10:25-10:45 Molecular-frame Momentum Imaging of Tunneling Electrons from Molecular Hydrogen in Circularly Polarized Intense Laser Fields

Hikaru Fujise (Nagoya Univ.)

10:45-11:05 3D-Visualization of Catalyst Materials and its Application to Infographic Approach

Hirosuke Matsui (Nagoya Univ.)

11:05-11:35 Dynamic Imaging of Electrochemical Reactions in All-Solid-State Li-Ion Batteries by Operando Scanning Transmission Electron Microscopy

Koh Saitoh (Nagoya Univ.)

11:35-11:45 Concluding Remarks

Ryotaro Matsuda (Nagoya Univ.)