

**First International Symposium of Institute for Catalysis  
– Global Collaboration in Catalysis Science toward Sustainable Society**

**October 13 (Tue.)**

----- **Plenary Lecture** -----

Chair: Kiyotaka Asakura

14:00 – 14:50     **Hans-Joachim Freund** (Fritz Haber Institute of the Max Planck Society)  
*Models for Heterogeneous Catalysts: Complex Materials at the Atomic Level*

Chair: Jun-ya Hasegawa

14:50 – 15:40     **Keiji Morokuma** (Kyoto University)  
*Theory and Computation Provide Insight and Discovery on Catalytic Reactions*

Chair: Atsushi Fukuoka

15:40 – 16:30     **Kazunari Domen** (University of Tokyo)  
*Development of Photocatalyst Sheets for Solar Hydrogen Production*

16:40 – 17:20     Ceremony

## October 14 (Wed.)

Chair: Satoru Takakusagi

- 9:00 – 9:30      **Jeffrey T. Roberts** (Purdue University)  
*Surface Modification of Aerosol Nanoparticles for Materials Applications*
- 9:30 – 9:50      **Bunsho Ohtani** (ICAT, Hokkaido University)  
*Fundamental Aspects on Heterogeneous Photocatalysis: Role of Electron Traps and Evidence for Multi-electron Transfer*
- 9:50 – 10:20     **Wataru Ueda** (Kanagawa University)  
*Catalysis Science in Crystalline Complex Metal Oxides*
- 10:20 – 10:40    **Ken-ichi Shimizu** (ICAT, Hokkaido University)  
*Cooperative Catalysis of Lewis Acid and Pt Nanoparticle for Reductive Transformations of Carboxylic Acids, Amides, and CO<sub>2</sub>*

Chair: Kiyotaka Nakajima

- 10:40 – 11:00    **Zhao-Xiong Xie** (Xiamen University)  
*Supersaturation Dependent Evolution of Nanocrystal Surfaces and Its Application in the Control of Surface Structure of Nanocatalysts*
- 11:00 – 11:20    **Atsushi Fukuoka** (ICAT, Hokkaido University)  
*Refrigerator Catalyst: Low-temperature Oxidation of Ethylene by Platinum supported on Mesoporous Silica*
- 11:20 – 11:50    **Bingjun Xu** (Delaware University)  
*Deciphering Complex Biomass Upgrade Processes on the Molecular Level*
- 11:50 – 12:10    **Ye Wang** (Xiamen University)  
*Selectivity Control in Catalytic Conversion of Synthesis Gas to Liquid Fuels*
- 12:10 – 13:30    ----- Lunch -----

Chair: Masamichi Ogasawara

- 13:30 – 14:00    **Fumiyuki Ozawa** (Kyoto University)  
*Palladium-Catalyzed Direct Arylation Polymerization (DARp): A Novel Synthetic Method of  $\pi$ -Conjugated Polymers*
- 14:00 – 14:20    **Tamaki Nakano** (ICAT, Hokkaido University)  
*Stereo-Controlled Polymers: Chiral Structure Regulation in the Ground and Excited States*

Chair: Tomohiro Yasuda

- 14:20 – 14:50    **Kazuyuki Tatsumi** (Nagoya University)  
*Reversible Transformation between Cuboidal Fe<sub>4</sub>S<sub>4</sub> and Dinuclear Fe<sub>2</sub>S<sub>2</sub> Cores*
- 14:50 – 15:10    **Tamotsu Takahashi** (ICAT, Hokkaido University)  
*Transformation of Organic Molecules on Titanium*
- 15:10 – 15:30    ----- Coffee Break -----

Chair: Shen Ye

15:30 – 16:00

**Li-Jun Wan** (University of Science and Technology of China)  
*Functional Electrode Materials and Solid/Liquid Interfacial Structure during Electrochemical Process*

16:00 – 16:30

**Masatoshi Osawa** (ICAT, Hokkaido University)  
*Water Molecules and Ions at Electrified Interfaces Studied by Surface-Enhanced Infrared Absorption Spectroscopy*

16:30 – 17:00

**Shi-Gang Sun** (Xiamen University)  
*In Situ FTIR Spectroscopic Studies of Electrocatalytic Reactions and Surface Processes*

Chair: Mayumi Nishida

17:00 – 17:30

**Kazuhiko Sato** (National Institute of Advanced Industrial Science)  
*Introduction of the Interdisciplinary Research Center for Catalytic Chemistry*

17:30 – 17:50

**Kiyotaka Asakura** (ICAT, Hokkaido University)  
*Quantum Beam and Catalysis Surface*

17:50 – 19:00

----- Poster Session -----

**October 15 (Thr.)**

***Special Session for “Bio-Interface”***

Chair: Ewa Kowalska

- 9:00 – 9:30      **Masaru Tanaka** (Kyushu University)  
*Design of Biocompatible Polymers Based on the Intermediate Water Concept*
- 9:30 – 10:10    **Elsa Yan** (Yale University)  
*Proteins at Interfaces Probed by Chiral Sum Frequency Generation Spectroscopy*
- 10:10 – 10:40   **Ichizo Yagi** (Hokkaido University)  
*Bio-inspired Electrocatalysts for Oxygen Reduction Reaction (ORR)*

Chair: Yasuhito Koyama

- 10:40 – 11:10   **Koichi Iwata** (Gakushuin University)  
*Lipid Bilayer Membranes as Field of Chemical Reactions – Characterization by Picosecond and Femtosecond Time-resolved Spectroscopy*
- 11:10 – 11:30   **Shen Ye** (ICAT, Hokkaido University)  
*Structure and Stability of Unsaturated Lipid Monolayer under Low-level of Ozone*
- 11:40 – 13:00   ----- Lunch -----

***Special Session for “Theory for Complex Systems”***

Chair: Akira Nakayama

- 13:00 – 13:30   **Kazunari Yoshizawa** (Kyushu University)  
*Quantum Chemical Studies on Dioxygen Activation and Methane Hydroxylation by Diiron and Dicopper Species as well as Related Metal–Oxo Species*
- 13:30 – 14:00   **Yoshitada Morikawa** (Osaka University)  
*Catalytic Reactions in Crystal Growth and Etching Processes at Semiconductor Surfaces: First-principles Molecular Dynamics Study*
- 14:00 – 14:30   **Hisao Nakamura** (National Institute of Advanced Industrial Science)  
*Computational Chemistry of Device Materials and Nano Interface Architectonics*

Chair: Hiroko Ariga

- 14:30 – 14:50   **Jun-ya Hasegawa** (ICAT, Hokkaido University)  
*Computational Chemistry toward Complex Molecular Systems*
- 14:50 – 15:10   **Akira Nakayama** (ICAT, Hokkaido University)  
*First-Principles Simulations of Oxygen Vacancy Transport at the Metal/Metal-Oxide Interface*
- 15:10 –            Closing Remarks