

Symposium S1, September 28 (Mon.) 16:20-19:40, Zoom 1

New aspects of excited-state properties of assemblies of metal complexes

Organizers:

Munetaka Iwamura (Toyama University)

16:20–16:25 **Opening remarks** Munetaka Iwamura (Toyama University)

Chair: Akitaka Ito (Kouchi University of Technology)

16:25–16:55 **S1-01** Helical Supramolecular Polymers formed via Self-Assembly of Diphenylisoxazole-Containing Small Aromatic Molecules
Takeharu Haino (Hiroshima University)

Chair: Kiyoshi Tsuge (Toyama University)

16:55–17:25 **S1-02** π – π stacking aggregation of anionic ligands, the photophysical properties, and the application to network formation
Masaki Kawano (Tokyo Institute of Technology)

Chair: Yusuke Kuramochi (Tokyo University of Science)

17:25–17:55 **S1-03** Luminescence color tuning of platinum(II) complex crystals induced by heating and mechanical grinding
Kazuteru Shinozaki (Yokohama City University)

17:55–18:00 **Break**

Chair: Kei Murata (Tokyo University)

18:00–18:30 **S1-04** Developments of Vapochromic Pt(II) Complexes for Visualization of Invisible Chemicals and Macroscopic Phenomena
Atsushi Kobayashi (Hokkaido University)

Chair: Michihiro Nishikawa (Tokyo University of Science)

18:30–19:00 **S1-05** Molecular Crystals of Gold Complexes with Unique Stimuli Responses
Tomohiro Seki (Hokkaido University)

Chair: Kiyoshi Miyata (Kyushu University)

19:00–19:30 **S1-06** Identification of Mettallophilic Oligomers in Aqueous Solution by Excited-state Vibration
Munetaka Iwamura (Toyama University)

19:30–19:40 **Closing remarks** Miki Hasegawa (Aoyama Gakuin University)

Symposium S2, September 28 (Mon.) 16:20-18:45, Zoom 2

Cooperative Interaction between Metal Atoms: Integrated Synthetic Methodology, Exploration of Unique Reactivity, and Theoretical Understanding of Metal Clusters

Organizers:

Hayato Tsurugi (Osaka University), Yasutaka Kitagawa (Osaka University)

16:20–16:25 **Opening remarks** Hayato Tsurugi (Osaka University)

Chair: Hayato Tsurugi (Osaka University)

16:25–16:50 **S2-01** Chiral Octapalladium Chains
Kanao Nakamae (Nara Women's University)

16:50–17:15 **S2-02** Theoretical study on metal-metal and metal-ligand interactions in polynuclear metal complexes
Yasutaka Kitagawa (Osaka University)

17:15–17:40 **S2-03** Coordination Behavior of Heteroarenes to Di- and Trinuclear Palladium Complexes
Koji Yamamoto (Tokyo Institute of Technology)

17:40–17:50 **Break**

Chair: Yasutaka Kitagawa (Osaka University)

17:50–18:15 **S2-04** Recent Progress in the Reaction Mechanism of Water-Splitting in Photosystem II
Mitsuo Shoji (University of Tsukuba)

18:15–18:40 **S2-05** Synthesis and Applications of Sterically Demanding Ferrocenyl Groups: d- π Electron Systems including Heavier Main Group Element
Takahiro Sasamori (Nagoya City University)

18:40–18:45 **Concluding remark** Yasutaka Kitagawa (Osaka University)

Symposium S3, September 28 (Mon.) 16:20-20:00, Zoom 3

New Era of Bioinorganic Chemistry Developed by the Quantum Beam and High Performance Computational Science

Organizers:

Takamitsu Kohzuma (Ibaraki University)

Chair: Takamitsu Kohzuma (Ibaraki University)

- 16:20–16:30 **S3-01** Study of Biomimetic Complexes of Galactose Oxidase: Influence of Weak Interaction of Second Coordination Sphere on the Electronic Structure of Active Site.
Hiromi Oshita (Konan University)
- 16:30–16:55 **S3-02** Complex Formation of Ni²⁺ with Acetonitrile, Methanol, and Dimethyl Sulfoxide in Imidazolium-based Ionic Liquids
Toshiyuki Takamuku (Saga University)
- 16:55–17:10 **S3-03** Structure Determination of the Open-Bundle Unfolding Intermediate of Cytochrome *c*' by Small Angle Neutron Scattering
Takahide Yamaguchi (Ibaraki University)
- 17:10–17:30 **S3-04** Formation of Cu^{II}-phenoxyl Radical by Reaction of O₂ with the Cu^{II}-Phenolate Complex via the Cu^I-Phenoxyl Radical Species
Yuichi Shimazaki (Ibaraki University)
- 17:30–18:05 **S3-05** J-PARC Muon Facility, MUSE
Yasuhiro Miyake (High Energy Accelerator Research Organization, KEK)
- 18:05–18:35 **S3-06** Neutron crystallography of copper amine oxidase: Novel hydrogen-bound and protonated structure in the active site
Toshihide Okajima (Osaka University)
- 18:35–18:45 **S3-07** Single-crystal Neutron Diffractometer iBIX at MLF, J-PARC
Katsuhiro Kusaka (Ibaraki University)
- 18:45–18:55 **S3-08** Possibility of a versatile neutron diffractometer, iMATERIA, in coordination chemistry
Akinori Hoshikawa (Ibaraki University)
- 18:55–19:10 **S3-09** Relationships between Protonation States around the Iron-Sulfur Cluster and the Function of 4Fe4S-type Ferredoxin Revealed by Neutron Crystallography
Masaki Unno (Ibaraki University)

- 19:10–19:25 **S3-10** Improved hydrogen evolution activity of the Ni-substituted rubredoxin by site-directed mutagenesis
Yasuhito Shomura (Ibaraki University)
- 19:25–19:45 **S3-11** Computational Insights into Chemical Reactions related to Coordination Chemistry
Seiji Mori (Ibaraki University)
- 19:45–20:00 **S3-12** Structural and Computational Studies of Weak Interactions at the Second Coordination Sphere in Blue Copper Protein, Pseudoazurin and its Met16X Variants
Attila Taborosi (Ibaraki University)

Symposium S4, September 28 (Mon.) 16:20-19:40, Zoom 4

New design of coordination geometries centered in solid state materials

Organizers:

Ryo Ohtani (Kyushu University), Kohei Yamagami (Okinawa Institute of Science and Technology Graduate University: OIST)

16:20–16:25 **Opening remarks** Ryo Ohtani (Kyushu University)

Chair: Ryo Ohtani (Kyushu University)

16:25–16:55 **S4-01** Migration and Condensation of Aqua Metal Ions Inside Metal Cluster Aggregates
Nobuto Yoshinari (Osaka University)

Chair: Tomoyo Misawa (Sophia University)

16:55–17:25 **S4-02** Solid-State High-Pressure Chemistry of Coordination Clusters: Structural Dynamics and Piezochromic Luminescence
Masaaki Abe (University of Hyogo)

Chair: Hiroyoshi Ohtsu (Tokyo Institute of Technology)

17:25–17:55 **S4-03** Controlling Local Structures of Mixed-anion Ceramics
Takafumi Yamamoto (Tokyo Institute of Technology)

17:55–18:05 **Break**

Chair: Takeshi Kitao (The University of Tokyo)

18:05–18:35 **S4-04** Porous Molecular Conductors: π -Radical-Based Self-Assembly for Constructing Electron-Conductive Coordination Networks
Hiroaki Iguchi (Tohoku University)

Chair: Fumiya Kobayashi (Tokyo University of Science)

18:35–19:05 **S4-05** Rotation of pillar ligands of MOFs and solid-state NMR analyses
Munehiro Inukai (Tokushima University)

Chair: Masami Yoshida (Hokkaido University)

19:05–19:35 **S4-06** Investigation of elemental-selective electronic states for transition-metal complexes in solids probed by X-ray absorption fine structure
Kohei Yamagami (OIST)

19:35–19:40 **Closing remarks** Kohei Yamagami (OIST)

Symposium S5, September 28 (Mon.) 16:20-19:35, Zoom 5

Advanced Functional Materials based on Polyoxometalates

Organizers:

Kosuke Suzuki (The University of Tokyo), Ryo Tsunashima (Yamaguchi University),
Sayaka Uchida (The University of Tokyo)

16:20–16:25 **Opening remarks** Kosuke Suzuki (The University of Tokyo)

Chair: Kosuke Suzuki (The University of Tokyo)

16:25–16:50 **S5-01** Structure Transformation of a Polyoxovanadate Molecular Container and Its Host-guest Property
Yuji Kikukawa (Kanazawa University)

16:50–17:15 **S5-02** Oxidation Catalysis over Crystalline Mo_3VO_x Catalysts
Satoshi Ishikawa (Kanagawa University)

17:15–17:40 **S5-03** Two-step Water Splitting by using Transition Metal-substituted Polyoxometalate as Shuttle Redox Mediator
Osamu Tomita (Kyoto University)

Chair: Ryo Tsunashima (Yamaguchi University)

17:40–18:05 **S5-04** Potentiality of Polyoxometalate Materials as Battery Electrodes
Hirofumi Yoshikawa (Kwansei Gakuin University)

18:05–18:15 **Break**

18:15–18:40 **S5-05** Development and Applications of a Single-molecule Electret Based on Polyoxometalate
Sadafumi Nishihara (Hiroshima University)

Chair: Sayaka Uchida (The University of Tokyo)

18:40–19:05 **S5-06** Polyoxometalate-based Gels for Solid-state Proton-conducting Supercapacitors
Hongying Zang (Northeast Normal University)

19:05–19:30 **S5-07** Exploring a Macroscopic Solid-state Property of Polyoxometalate-based Hybrids
Ryo Tsunashima (Yamaguchi University)

19:30–19:35 **Closing remarks** Sayaka Uchida (The University of Tokyo)