Fri., Jan. 25

12:30	Registration
13:30	Opening Remarks
13:40	**[YR-1] Zhang** *Nagoya Univ.*
14:00	**[SR-1] Okada** *Kyushu Univ.*
14:30	**[YR-2] Hirose** *Kyoto Univ.*
14:50	Coffee break
15:10	**[SR-2] Wakamiya** *Kyoto Univ.*
15:40	**[IL-1] Yeh** *National Sun Yat-sen Univ.*
16:30	Poster Session odd #: former even #: latter
18:00	Banquet
20:00	

Sat., Jan. 26

9:20	**[SR-3] Ohtani** *Hokkaido Univ.*
9:50	**[IL-2] Tachibana** *RMIT Univ.*
10:30	Coffee break
10:50	**[YR-3] Igawa** *Kyushu Univ.*
11:10	**[SR-4] Yamaguchi** *Nagoya Univ.*
11:40	**[YR-4] Toyao** *Hokkaido Univ.*
12:00	Lunch
13:20	**[IL-3] Kim** *Ewha Womans Univ.*
14:00	**[IL-4] Durrant** *Imperial College London*
14:50	Closing Remarks

IRCCS The 2nd International Symposium

"New Future by Chemical Synthesis and Energy Materials"

Jan. 25th–26th, 2019

Kihada Hall, Uji Campus, Kyoto University, Uji Japan

January 25th (Fri.)

12:30–13:30	Registration
13:30–13:40	Opening Remarks
13:40–14:00	*(Chair: Masaharu Nakamura, Kyoto University)* [YR-1] **Zhongyue Zhang** (*Nagoya University, Japan*) "Triptycene-Derived Metal-Organic Frameworks: Unusual Topologies, Connectivites and Physical Properties"
14:00–14:30	[SR-1] **Shigeto Okada** (*Kyushu University, Japan*) "High Voltage Sodium-Ion Battery by Concentrated Aqueous Electrolyte"
14:30–14:50	[YR-2] **Takashi Hirose** (*Kyoto University, Japan*) "Development of Molecular Functions Based on Helically Twisted Polycyclic Aromatic Hydrocarbons"
14:50–15:10	Coffee break
15:10–15:40	*(Chair: Yasujiro Murata, Kyoto University)* [SR-2] **Atsushi Wakamiya** (*Kyoto University, Japan*) "Purified Materials for Highly Efficient Perovskite Solar Cells"
15:40–16:30	[IL-1] **Wen-Yann Yeh** (*National Sun Yat-sen University, Taiwan*) "Metal Complexation and C–C Bond Activation with Fullerenes"
16:30–18:00	Poster session at 2nd floor The former half: odd numbers, the latter half: even numbers.
18:00–20:00	Banquet (Kihada restaurant, 2nd floor)

January 26th (Sat.)

(Chair: Hideki Hirori, Kyoto University)

09:20–09:50 [SR-3] **Bunsho Ohtani** (*Hokkaido University, Japan*)
"Identification and Detailed Characterization of Metal-Oxide Powders with Their Energy-Resolved Distribution of Electron Traps"

09:50–10:30 [IL-2] **Yasuhiro Tachibana** (*RMIT University, Australia*)
"Interfacial Charge Transfer and Transport Dynamics in Lead Halide Perovskite Solar Cells"

10:30–10:50 Coffee break

(Chair: Yoshiyuki Mizuhata, Kyoto University)

10:50–11:10 [YR-3] **Kazunobu Igawa** (*Kyushu University, Japan*)
"Stereoselective Synthesis of Asymmetric Silicon Molecules"

11:10–11:40 [SR-4] **Shigehiro Yamaguchi** (*Nagoya University, Japan*)
"Phosphorus-Containing Photostable and NIR Fluorophores for Bio-Imaging"

11:40–12:00 [YR-4] **Takashi Toyao** (*Hokkaido University, Japan*)
"Statistical Analysis and Design of Heterogeneous Catalysis Using Machine Learning"

12:00–13:20 Lunch

(Chair: Atsushi Wakamiya, Kyoto University)

13:20–14:00 [IL-3] **Kyungkon Kim** (*Ewha Womans University, Korea*)
"Strategies to Enhance the Performance and Stability of Organic Photovoltaics"

14:00–14:50 [IL-4] **James Durrant** (*Imperial College London, UK*)
"Charge Carrier Dynamics in Conjugated Polymers for Organic Solar Cells and Solar to Fuels"

14:50–15:00 Closing Remarks

Poster Session

At 2nd floor, from 16:30 to 18:00 on January 25th (Fri.).
The posters with odd numbers will be presented in the former half and even numbers in the latter half.
After this session, please remove posters by 12:00 on January 26th (Sat.).

[P-1] Hiroe Kubota, Takehiro Amada, Takashi Toyao, Zen Maeno, Ken-ichi Shimizu
"Spectroscopic and Theoretical Investigations of the Mechanism of NH_3-SCR Reactions over Cu-Zeolite Catalysts"

[P-2] Shunsaku Yasumura, Liu Chong, Takashi Toyao, Zen Maeno, Ken-ichi Shimizu
"Theoretical Investigation of 13-Group Metal Clusters in CHA Zeolite by Ab Initio Thermodynamics Analysis"

[P-3] Fitri Rizki Amalia, Mai Takashima, Bunsho Ohtani
"Development of a Simple but Reliable Method for Photocatalytic-Activity Evaluation"

[P-4] Pradudnet Ketwong, Shugo Takeuchi, Mai Takashima, Bunsho Ohtani
"Light Intensity-Dependence Study for Titania Photocatalysis with Multielectron Transfer Processes"

[P-5] Tharishinny Raja Mogan, Mai Takashima, Ewa Kowalska, Bunsho Ohtani
"Synthesis of Gold-Nanoparticle/silica Colloidal Crystal to Form Highly Ordered Titania Inverse-Opal Structures"

[P-6] Nabin Ch. Maity, Maximilian Krämer, Jun-ya Hasegawa, Tamaki Nakano
"Synthesis and Characterization of a Novel Fluorenone Derivative with Intramolecular Charge Transfer Properties"

[P-7] Maia Merlani, Vakhtang Barbakadze, Zhiyi Song, Tamaki Nakano
"Studies on Synthetic Analogues of Comfrey-Based, Wound-Healing Natural Biopolymer"

[P-8] Nino Zavradashvili, Yue Wang, Zhiyi Song, Ramaz Katsarava, Tamaki Nakano
"Synthesis and Physicochemical Properties of Chiral Cationic Polymers"

[P-9] Kashaboina Upendar, Natee Sirisit, Hiroko Ariga-Miwa, Satoru Takakusagi, Yuta Nishikawa, Fumiya Kuriyama, Arnoldus lambertus Dipu, Hitoshi Ogiwara, Shoji Iguchi, Ichiro Yamanaka, Takahiro Wada, Kiyotaka Asakura
"Operando EXAFS Analysis of In/SiO_2 Catalyst during NMC"

[P-10] Min Gao, Andrey Lyalin, Satoshi Maeda, Tetsuya Taketsugu
"Theoretical Study on Geometry Effect on the Catalytic Activity of Gold Clusters"

[P-11] Toshiyuki Sugiyama, Akira Nakayama, Jun-ya Hasegawa
"Reaction Mechanism of the Direct Synthesis of Dimethyl Carbonate from CO_2 and Methanol over Metal-Oxide Catalysis: a Theoretical Study"

[P-12] Liming Zhao, Akira Nakayama, Koji Oohora, Hiroyuki Meichin, Takashi Hayashi, Jun-ya Hasegawa
"Controlled Intersystem Crossing in Iron Porphycene Substituted Myoglobin for Cyclopropanation Reaction: a Theoretical Study"

[P-13] Pengru Chen, Abhijit Shrotri, Atsushi Fukuoka
"Selective Synthesis of Cello-Oligosaccharides by Hydrolysis of Cellulose over Carbon Catalyst in a Semi-Flow Reactor"

[P-14] Kyohei Tomita, Shin-ichiro Kawano, Kentaro Tanaka
"Development of Columnar Liquid Crystals of Macrocycles toward Anisotropic Transport of Lithium Ion"

[P-15] Masaaki Saitow
"Accurate Wave Function Theories for Large, Real-life Molecules"

[P-16] Ryosuke Y. Shimizu, Takeshi Yanai, Yuki Kurashige, Daisuke Yokogawa
"Calculating Bioimaging Probes with RISM(-DMRG)-CASPT2"

[P-17] Ayaka Yoshikawa, Masaaki Saitow, Takeshi Yanai
"A Hybrid Solvation Model Using CPCM in CASSCF Framework for Real-Life Molecules"

[P-18] Ayano Yamada, Masaaki Saitow, Takeshi Yanai
"Development of Fast and Accurate Self-Consistent Field Method Based on Local Resolution-of-the-Identity Approximation"

[P-19] Ayaka Ueda, Hiroyuki Kitano, Jaehoon Choi, Hideto Ito, Shinya Hagihara, Toshiyuki Kan, Hirokazu Kawagishi, Kenichiro Itami
"Discovery of Plant Growth Stimulants by C–H Arylation of 2-Azahypoxanthine"

[P-20] Shusei Fujiki, Akiko Yagi, Kenichiro Itami
"Solid-Phase Synthesis of Unsubstituted Poly(*para*-phenylene)"

[P-21] Asuka Naraoka, Tomoya Kanda, Hiroshi Naka
"Palladium-Catalyzed Transfer Hydration of Cyanohydrins"

[P-22] Shota Yoshioka, Masayuki Naruto, Ke Wen, Susumu Saito
"Development of Bidentate Diphosphine Ligands of Highly Active Ru Catalysts for Practical Hydrogenation of Carboxylic Acids"

[P-23] Yuma Sasaki, Hikaru Fujise, Yoshitaka Kawabe, Kasumi Hashigaya, Akitaka Matsuda, Yasumasa Hikosaka, Mizuho Fushitani, Akiyoshi Hishikawa
"Formation of Xe 4d Double-Core-Hole States in Strong XUV-FEL Fields Studied by Electron-Ion Coincidence Spectroscopy"

[P-24] Kouhei Wakamatsu, Hirosuke Matsui, Nozomu Ishiguro, Satoshi Muratsugu, Mizuki Tada
"*In situ* XAFS Imaging of Redox-Active Ceria Particles with Transition Metals"

[P-25] Kodai Ishihara, Yuna Araki, Mizuki Tada, Yoichi Sakai, Yasuhiro Ohki
"Synthesis of Dinuclear Mo-Fe Hydride Complexes for the Catalytic Silylation of N_2"

[P-26] Yusaku Kodama, Shinya Ariyasu, Osami Shoji, Yoshihito Watanabe
"Direct Hydroxylation of Gaseous Alkane by Cytochrome P450 under High-Pressure Condition"

[P-27] Yuichiro Aiba, Masaki Hibino, Gerardo Urbina, Yuuki Ochiai, Naomi Kochi, Masanari Shibata, Osami Shoji, Yoshihito Watanabe
"Chemically-Modified Peptide Nucleic Acids for *in cellulo* Applications"

[P-28] Hideo Katakura, Yushi Niimi, Fumiaki Tomoike, Yasuaki Kimura, Hiroshi Abe
"Development of 2′-Modified Nucleoside Analogues as Antiviral Agents"

[P-29] Haruka Fujikawa, Yuko Shishido, Keiko Kuwata, Yasuaki Kimura, Fumiaki Tomoike, Hiroshi Abe
"A Covalent Inhibitor for Glutathione *S*-Transferase Pi (GSTP1-1) in Human Cells"

[P-30] Qing Wang, Marek Grzybowski, Masayasu Taki, Shigehiro Yamaguchi
"Phospha-Rhodamine based Glutathione Fluorescent Probes"

[P-31] Yoshiaki Sugihara, Shigehiro Yamaguchi
"Donor–π–Acceptor-Type Boron-Containing NIR-Fluorophores"

[P-32] Yoshiaki Shuku, Kunio Awaga
"Honeycomb Crystal Structures Formed by 3-Fold Symmetric Triptycene Derivatives"

[P-33] Dongwan Yan, Yang Wu, Kunio Awaga
"Highly-Porpous Heteroatom-Doped Carbons Prepared by Salt-Assisted Pyrolysis of Covalent Organic Frameworks for High-Performance Supercapacitors"

[P-34] Tomoko Aharen, Taketo Handa, Takumi Yamada, Atsushi Wakamiya, Yoshihiko Kanemitsu
"Lead-Free Halide Perovskites: Effect of Additive Choice and Solvent Engineering on Optical Properties and Cell Performance"

[P-35] Yasuyuki Sanari, Tomohito Otobe, Yoshihiko Kanemitsu, Hideki Hirori
"Nonlinear Interaction of Strong Laser Fields with Semiconducting Materials in the Nonperturbative Regime"

[P-36] Takumi Yamada, Tomoko Aharen, Yoshihiko Kanemitsu
"Anti-Stokes Photoluminescence Properties of Lead-Halide Perovskite Semiconductors"

[P-37] Keiichi Ohara, Takumi Yamada, Hirokazu Tahara, Tomoko Aharen, Hideki Hirori, Yoshihiko Kanemitsu
"Nonlinear Optical Properties of Lead Halide Perovskite Single Crystals"

[P-38] Sojiro Masada, Naoki Yarita, Hirokazu Tahara, Masaki Saruyama, Tokuhisa Kawawaki, Ryota Sato, Toshiharu Teranishi, Yoshihiko Kanemitsu
"Photoluminescence Properties of Lead Bromide Perovskites Nanocrystals Revealed by Single-Dot Spectroscopy"

[P-39] Satoshi Nakahara, Hirokazu Tahara, Go Yumoto, Tokuhisa Kawawaki, Masaki Saruyama, Ryota Sato, Toshiharu Teranishi, Yoshihiko Kanemitsu
"Mechanism of Trion Generation in $CsPbBr_3$ Perovskite Nanocrystals"

[P-40] Hirokazu Tahara, Masanori Sakamoto, Toshiharu Teranishi, Yoshihiko Kanemitsu
"Coherent Spectroscopy of Multiple Excitons in Semiconductor Nanocrystals"

[P-41] Taketo Handa, Tomoko Aharen, Atsushi Wakamiya, Yoshihiko Kanemitsu
"Fundamental Optical Responses of Lead-Free Tin Iodide Perovskites"

[P-42] Hideki Hirori
"Crystallization of Phase-Change Materials Induced by Strong THz Pulses"

[P-43] Jing-Dong Guo, Tomohiro Sugahara, Takahiro Sasamori, Shigeru Nagase, Norihiro Tokitoh
"Mechanistic Studies on Reversible Addition of Terminal Alkene to Digermynes"

[P-44] Tomohiro Sugahara, Takahiro Sasamori, Norihiro Tokitoh
"Synthesis and Properties of 2,5-Digermaselenophene"

[P-45] Shiori Fujimori, Yoshiyuki Mizuhata, Norihiro Tokitoh
"Synthesis and Structure of Heavier Group 14 Element Analogues of Aryl Anions"

[P-46] Jiewei Liu, Masashi Ozaki, Shinya Yakumaru, Taketo Handa, Ryosuke Nishikubo, Yoshifumi Hashikawa, Yasujiro Murata, Takashi Saito, Yuichi Shimakawa, Yoshihiko Kanemitsu, Akinori Saeki, Richard Murdey, Atsushi Wakamiya
"Simple Approaches to Realize Efficient and Reproducible Lead-free Perovskite Solar Cells: Purification of Precursor Materials and Modification of Solution Process"

[P-47] Minh Anh Truong, Richard Murdey, Atsushi Wakamiya
"Transparent Hole-Transporting Materials Containing Partially Oxygen-Bridged Triphenylamine Skeletons: Synthesis and Properties"

[P-48] Sheng Zhang, Yoshifumi Hashikawa, Yasujiro Murata
"Cage-Expansion of Fullerene from C_{60} to $C_{65}N$ and $C_{64}N$ Skeletons"

[P-49] Shota Hasegawa, Yoshifumi Hashikawa, Yasujiro Murata
"Dynamic Behavior of a Single H_2O Molecule Induced by Hydrogen-Bondings inside an Open-Cage Fullerene C_{60} Derivative"

[P-50] Francesca Pincella, Katsuhiro Isozaki, Hikaru Takaya, Masaharu Nakamura
"Magnetic Iron Oxide Nanoparticles as Green and Recyclable Catalysts for the Selective Microwave-Assisted Oxidation of Secondary Alcohols"

[P-51] Atsushi Hosokawa, Takahiro Iwamoto, Masaharu Nakamura
"Light-Driven Entropically Unfavourable Coupling between *N*-Methylamine and Aromatic Ketone"

[P-52] Takafumi Shanoh, Hikaru Takaya, Masato Ito, Masaharu Nakamura
"Synthetic Resolution of Wood Lignin by Iron-Catalyzed Oxidation"

[P-53] Anucha Koedtruad, Taketo Handa, Tomoya Nakamura, Takashi Saito, Daisuke Kan, Yoshihiko Kanemitsu, Atsushi Wakamiya, Yuichi Shimakawa
"Crystal Structures and Properties of Ag-Bi-I Compounds"

[P-54] Yooun Heo, Daisuke Kan, Yuichi Shimakawa
"Dynamics of Oxygen Ions in $SrFeO_{2.5+\delta}$ Thin Films"

[P-55] Zhenhong Tan, Takashi Saito, Fabio Denis Romero, Midori Amano Patino, Masato Goto, Yuichi Shimakawa
"Novel Hexagonal Perovskite $Ba_4Fe_3NiO_{12}$ Containing Tetravalent Fe and Ni Ions"

[P-56] Pritam Sadhukhan, Shengqun Su, Shinji Kanegawa, Osamu Sato
"Directional Electron Transfer Coupled Spin-Crossover in the Crystals of [FeCo] Di-Nuclear Complexes Facilitating Ultrafast Polarization Switching"

[P-57] Sheng-qun Su, Shu-qi Wu, Shinji Kanegawa, Osamu Sato
"Tetrahydrofuran-Triggered Magnetic Coupled with Vapochromism Switching in a Cobalt(II)-Based Single-Ion Magnet"

[P-58] Tsukasa Abe, Yuta Hori, Yoshihito Shiota, Kazunari Yoshizawa
"Aldol Reaction Type C–C Bond Formation Catalyzed by a Mononuclear Copper(II)-Superoxide Complex"

[P-59] Yuuya Kawasaki, Yuuki Seto, Shintarou Kawahara, Kazunobu Igawa, Katsuhiko Tomooka
"Development and Application of Multi-Molecule Connectable DACN"

[P-60] Takayuki Iwata, Takuto Fukami, Tatsuro Yoshinaga, Takumi Fujiwara, Mitsuru Shindo
"Synthesis of Iptycenes Using Ynolate-Aryne Triple Cycloaddition"

[P-61] Shinji Kanegawa, Osamu Sato
"Polarity Switching Crystals Prepared by Pseudo-Racemic Crystallization"

[P-62] Takumi Nakanishi, Osamu Sato
"Proton Coupled Spin Transition in Fe(II) Coordination Compounds"

[P-63] Takuro Hosomi, Kazuki Nagashima, Tsunaki Takahashi, Nobutaka Shioya, Takafumi Shimoaka, Guozhu Zhang, Masaki Kanai, Takeshi Hasegawa, Takeshi Yanagida
"Regioselective Oxidation of Aliphatic Ketones on ZnO Single-Crystal Nanowires"

[P-64] Kei Ikeda, Yuta Hori, Yoshihito Shiota, M. Haris Mahyuddin, Aleksandar Staykov, Takahiro Matsumoto, Kazunari Yoshizawa, Seiji Ogo
"Theoretical Study of H_2O Oxidation by a Half-Sandwich Iridium Complex"

[P-65] Kazuki Nagashima, Hirotaka Koga, Tsunaki Takahashi, Masaya Nogi, Takeshi Yanagida
"Robust Nanowire-Nanocellulose Composite Network Structure for One-Time Use Disposable Paper Molecular Sensor"

[P-66] Takeru Torigoe, Ryuhei Muta, Yoichiro Kuninobu
"Regioselective Trifluoromethylthiolation of *N*-Heteroaromatic Compounds"

[P-67] Yuta Tsuji, Kaunzari Yoshizawa
"Effects of Electron-Phonon Coupling on Quantum Interference in Polyenes"

[P-68] Atsushi Tahara, Yuto Ii, Yusuke Sunada, Mitsunobu Kawamura, Hideo Nagashima
"Reverse ATRP of St and MMA Catalyzed by $Me_3TACNFeX_3$ (X = Cl, Br)"

[P-69] Yuta Hori, Takumi Nakanishi, Yoshihito Shiota, Osamu Sato, Kazunari Yoshizawa
"Theoretical Study of Proton-Coupled Spin Crossover Fe(II) Complexes"

[P-70] Yuki Yoshida, Kouhei Machida, Mariko Okamoto, Yusuke Ano, Kazunobu Igawa, Katsuhiko Tomooka
"Photochemical Isomerization Approach to Planar Chiral Medium-Sized Cyclic Molecules"