

# JULY 28 FRI

ROOM A	ROOM B	ROOM C	ROOM D
<p>Chair : Dominik Wöll and Tsukasa Torimoto</p>			
<p><b>9:00 AM - 9:45 AM</b> [PL11] Materials Design for Implementing High Voltage Perovskite Solar Cells *Tsutomu Miyasaka<sup>1</sup> (1. Toin Univ. of Yokohama (Japan))</p>			
<p>Chair : Dominik Wöll and Tsukasa Torimoto</p>			
<p><b>9:45 AM - 10:30 AM</b> [PL12] Development of Exciton Processes Aimed at High-Performance TADF and Hyperfluorescence OLEDs *Chihaya Adachi<sup>1</sup> (1. Kyushu Univ. (Japan))</p>			
<p style="text-align: center;"><b>BREAK</b></p>		<p style="text-align: center;"><b>BREAK</b></p>	
<p>Chair : Ayumi Ishii</p>	<p>Chair : Hisanao Usami</p>	<p>Chair : Kyung-Ryang Wee</p>	<p>Chair : Yasutaka Kitagawa</p>
<p><b>11:00 AM - 11:15 AM</b> [S9-13-CL] Binaphthalimide motif as chiral scaffold for thermally activated delayed fluorescence and circularly polarized luminescence activity *Marine Louis<sup>1</sup>, Yugo Tsuji<sup>1</sup>, Natsuko Kanno<sup>2</sup>, Katsuyuki Shizu<sup>2</sup>, Hironori Kaji<sup>2</sup>, Tsuyoshi Kawai<sup>1</sup> (1. Nara institute of Science and Technology (Japan), 2. Kyoto Univ. (Japan))</p>	<p><b>11:00 AM - 11:15 AM</b> [S5-20-CL] Strategies to enhance the photostability of coordination complexes, from single molecule to complex materials *Pau Farràs<sup>1</sup>, Roberto Gonzalez-Gomez<sup>1</sup>, Sean Hennessey<sup>1</sup> (1. Univ. of Galway (Ireland))</p>	<p><b>11:00 AM - 11:15 AM</b> [S6-13-CL] Morphology-Controlled Synthesis of Metalloporphyrin Coordination Polymer Particles (CPPs) for Photocatalytic Reactions and its Trace -Identification by Surface Enhanced Raman Spectroscopy (SERS) *Yu Sun<sup>1</sup> (1. Hokkaido Univ. (Japan))</p>	<p><b>11:00 AM - 11:25 AM</b> [S8-01-KL] Explaining, Predicting and Discovering Photochemistry from First Principles *Todd Martinez<sup>1,2</sup> (1. Stanford Univ. (USA), 2. SLAC National Accelerator Laboratory (USA))</p>
<p>Chair : Ayumi Ishii</p>	<p>Chair : Hisanao Usami</p>	<p>Chair : Kyung-Ryang Wee</p>	<p>Chair : Yasutaka Kitagawa</p>
<p><b>11:15 AM - 11:30 AM</b> [S9-14-CL] Human brain tumor diagnosis using luminescent Eu(III) complex *Mengfei Wang<sup>1,3</sup>, Masaya Kono<sup>2</sup>, Yusaku Yamaguchi<sup>2</sup>, Sunao Shoji<sup>1,3</sup>, Yuichi Kitagawa<sup>1,3</sup>, Koji Fushimi<sup>3</sup>, Masumi Tsuda<sup>1,4</sup>, Shinya Tanaka<sup>1,4</sup>, Yasuchika Hasegawa<sup>1,3</sup> (1. Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido Univ. (Japan), 2. Grad. Sch. of Chem. Sci. and Eng., Hokkaido Univ. (Japan), 3. Fac. of Eng., Hokkaido Univ. (Japan), 4. Fac. of Med., Hokkaido Univ. (Japan))</p>	<p><b>11:15 AM - 11:30 AM</b> [S5-21-CL] Red-light-driven CO<sub>2</sub> reduction using an osmium complex as a panchromatic self-photosensitized catalyst *Jieun Jung<sup>1</sup>, Kenji Kamada<sup>1</sup>, Susumu Saito<sup>1,2</sup> (1. Graduate School of Science, Nagoya Univ. (Japan), 2. Integrated Research Consortium on Chemical Sciences, Nagoya Univ. (Japan))</p>	<p><b>11:15 AM - 11:30 AM</b> [S6-14-CL] The electron donating behavior of DMSO in the excited state intermolecular proton transfer reaction of pyrene-urea compounds *Leyun Huang<sup>1</sup>, Mayu Yoshida<sup>1</sup>, Yoshinobu Nishimura<sup>1</sup> (1. Univ. of Tsukuba (Japan))</p>	<p><b>11:25 AM - 11:40 AM</b> [S8-02-CL] Modeling ultrafast charge-transfer in organic photovoltaic materials from first-principles: the role of quantum vibrations, environment disorder and light pulse shape *Elisa Palacino Gonzalez<sup>1</sup>, Thomas la Cour Jansen<sup>1</sup> (1. Univ. of Groningen (Netherlands))</p>

# JULY 28 FRI

ROOM A	ROOM B	ROOM C	ROOM D
<p style="text-align: right;">Chair : Ayumi Ishii</p> <p><b>11:30 AM - 11:45 AM</b> <b>[S9-15-CL]</b> Development of Indigos as Red-Light Photoswitches *Chung-Yang (Dennis) Huang<sup>1</sup>, Amit Kumar Jaiswal<sup>1</sup>, Priya Saha<sup>1</sup>, Anna Jasny<sup>2</sup>, Stefan Hecht<sup>2</sup> (1. ICRReDD, Hokkaido University (Japan), 2. Humboldt Univ. at Berlin (Germany))</p> <p style="text-align: right;">Chair : Ayumi Ishii</p> <p><b>11:45 AM - 12:00 PM</b> <b>[S9-16-CL] Cancelled</b></p>	<p style="text-align: right;">Chair : Hisanao Usami</p> <p><b>11:30 AM - 11:55 AM</b> <b>[S5-22-KL]</b> Mixed-Anion Photocatalysts for Visible-Light-Induced Water Splitting *Ryu Abe<sup>1</sup> (1. Kyoto Univ. (Japan))</p>	<p style="text-align: right;">Chair : Kyung-Ryang Wee</p> <p><b>11:30 AM - 11:45 AM</b> <b>[S6-15-CL]</b> Polymetallic Ir(III) and Ru(II) Photosensitisers for Photoredox Catalysed Organic Transformation Reactions *Tara Kelly Davids<sup>1</sup>, Nozuko Motimani<sup>2</sup>, Siyabonga Ngubane<sup>3</sup>, Wade Petersen<sup>4</sup>, Gregory Smith<sup>5</sup> (1. Univ. of Cape Town (South Africa), 2. Univ. of Cape Town (South Africa), 3. Univ. of Cape Town (South Africa), 4. Univ. of Cape Town (South Africa), 5. Univ. of Cape Town (South Africa))</p> <p style="text-align: right;">Chair : Kyung-Ryang Wee</p> <p><b>11:45 AM - 12:05 PM</b> <b>[S6-16-IL]</b> High-yield triplet exciton generation through singlet fission for efficient light energy conversion *Taku Hasobe<sup>1</sup> (1. Faculty of Science and Technology, Keio Univ. (Japan))</p>	<p style="text-align: right;">Chair : Yasutaka Kitagawa</p> <p><b>11:40 AM - 11:55 AM</b> <b>[S8-03-CL]</b> Photochemistry, photophysics and spectroscopy using high-dimensional quantum wave packets and <i>ab initio</i> potential energy surfaces *David Picconi<sup>1</sup> (1. Zernike Institute for Advanced Materials, Univ. of Groningen (Netherlands))</p> <p style="text-align: right;">Chair : Yasutaka Kitagawa</p> <p><b>11:55 AM - 12:10 PM</b> <b>[S8-04-CL]</b> Excited-state density functional tight-binding for simulation and virtual screening of molecular photophysical properties Megan Y. Deshayes<sup>1</sup>, Zoe A. Pollard<sup>1</sup>, Gunnar J. Carlson<sup>1</sup>, Alex T. Wrede<sup>1</sup>, Reuben A. Szabo<sup>1</sup>, *Tim Kowalczyk<sup>1</sup> (1. Western Washington Univ. (USA))</p>
<b>LUNCH BREAK</b>		<b>LUNCH BREAK</b>	
<p style="text-align: right;">Chair : Vincent Chi-Chiu Ko and Yasuchika Hasegawa</p> <p><b>1:30 PM - 1:45 PM</b> <b>[S9-17-CL]</b> Up-conversion Induced Near-infrared Light Detection in Lead Halide Perovskite with Core-shell Lanthanide Nanoparticles *Ayumi Ishii<sup>1</sup> (1. Waseda Univ. (Japan))</p>	<p style="text-align: right;">Chair : Shigeyuki Masaoka and Wei-Yin Sun</p> <p><b>1:30 PM - 1:45 PM</b> <b>[S5-23-CL]</b> Solar fuel production by photo-redox-cascade catalyst composing dual photosensitizers and transparent hole acceptor *Atsushi Kobayashi<sup>1</sup>, Nobutaka Yoshimura<sup>1</sup>, Masaki Yoshida<sup>2</sup> (1. Hokkaido Univ. (Japan), 2. Kwansei Gakuin Univ. (Japan))</p>	<p style="text-align: right;">Chair : Yu Sun and Yoshinobu Nishimura</p> <p><b>1:30 PM - 1:50 PM</b> <b>[S6-17-IL]</b> Development of Stable Dye-sensitized Photoelectrosynthesis Cell by Electropolymerization Strategy for Solar Fuel Production *Kyung-Ryang Wee<sup>1</sup> (1. Daegu Univ. (Korea))</p>	<p style="text-align: right;">Chair : Miho Hatanaka</p> <p><b>1:30 PM - 1:45 PM</b> <b>[S8-05-CL]</b> <i>In silico</i> frontier orbital energy design of photosensitizer by multivariate analysis and density functional theory calculation *Yasutaka Kitagawa<sup>1,2,3,4,5</sup>, Kazuaki Tokuyama<sup>1</sup>, Hiromasa Sato<sup>1</sup>, Mitsuhiro Nishida<sup>1</sup>, Naoka Amamizu<sup>1</sup>, Yuta Hayashi<sup>1</sup>, Keisuke Sasaki<sup>1</sup>, Masahiro Tsuda<sup>1</sup>, Ryohei Kishi<sup>1,2,3,5</sup> (1. Graduate School of Engineering Science, Osaka Univ. (Japan), 2. IQIB, Osaka Univ. (Japan), 3. ICS-OTRI, Osaka Univ. (Japan), 4. SRN-OTRI, Osaka Univ. (Japan), 5. RCSEC, Osaka Univ. (Japan))</p>

# JULY 28 FRI

## ROOM A

Chair : Vincent Chi-Chiu Ko and  
Yasuchika Hasegawa

### 1:45 PM - 2:00 PM

**[S9-18-CL]** Paper-based fluorescent microarray devices for pattern recognition-driven chemical sensing

\*Tsuoyoshi Minami<sup>1</sup> (1. Univ. of Tokyo (Japan))

Chair : Vincent Chi-Chiu Ko and  
Yasuchika Hasegawa

### 2:00 PM - 2:15 PM

**[S9-19-CL]** Metal Acyclic Carbene Complexes: Luminescent Mechanochromism and Applications

\*Vincent Chi-Chiu Ko<sup>1</sup> (1. Department of Chemistry, City Univ. of Hong Kong (Hong Kong))

Chair : Vincent Chi-Chiu Ko and  
Yasuchika Hasegawa

### 2:15 PM - 2:35 PM

**[S9-20-IL]** Tunable Optical Properties of Less-toxic Multinary Quantum Dots Composed of Ag–In–Ga–S Alloys and Related Compounds

\*Tsukasa Torimoto<sup>1</sup>, Tatsuya Kameyama<sup>1</sup>, Taro Uematsu<sup>2</sup>, Susumu Kuwabata<sup>2</sup> (1. Graduate School of Engineering, Nagoya Univ. (Japan), 2. Graduate School of Engineering, Osaka Univ. (Japan))

## ROOM B

Chair : Shigeyuki Masaoka and Wei-Yin Sun

### 1:45 PM - 2:00 PM

**[S5-24-CL]** Enhancing Electrocatalytic Oxygen Reduction Reaction through Laser Excitation of Plasmonic Metal – Semiconductor Metal Oxide Heterojunctions

\*Joey Andrew Arquisola Valinton<sup>1</sup>, Min-Chuan Chung<sup>1</sup>, Wei-Quan Chen<sup>1</sup>, Chun-Hu Chen<sup>1</sup> (1. National Sun Yat-sen Univ. (Taiwan))

Chair : Shigeyuki Masaoka and Wei-Yin Sun

### 2:00 PM - 2:15 PM

**[S5-25-CL]** Multi-dentate Coordination of Triethanolamine to Zn Porphyrin and Re Complex Enhancing Photocatalytic CO<sub>2</sub> Reduction

\*Yusuke Kuramochi<sup>1</sup>, Yuto Suzuki<sup>1</sup>, Akiharu Satake<sup>1</sup> (1. Tokyo Univ. of Science (Japan))

Chair : Shigeyuki Masaoka and Wei-Yin Sun

### 2:15 PM - 2:35 PM

**[S5-26-IL]** Development of Molecular Catalysts for Photosynthetic Reactions

\*Shigeyuki Masaoka<sup>1</sup> (1. Osaka Univ. (Japan))

## ROOM C

Chair : Yu Sun and Yoshinobu Nishimura

### 1:50 PM - 2:05 PM

**[S6-18-CL]** Photoexcited charge manipulation in  $\pi$ -conjugated polymers bearing metal-complex catalysts for visible-light CO<sub>2</sub> reduction

\*Akinobu Nakada<sup>1,2</sup>, Chen Zhang<sup>1</sup>, Ryuichi Miyakawa<sup>3</sup>, Hajime Suzuki<sup>1</sup>, Kosaku Kato<sup>4</sup>, Akinori Saeki<sup>5</sup>, Akira Yamakata<sup>4</sup>, Hiromi Nakai<sup>6</sup>, Ho-Chol Chang<sup>3</sup>, Ryu Abe<sup>1</sup> (1. Kyoto Univ. (Japan), 2. PRESTO/JST (Japan), 3. Chuo Univ. (Japan), 4. Okayama Univ. (Japan), 5. Osaka Univ. (Japan), 6. Waseda Univ. (Japan))

Chair : Yu Sun and Yoshinobu Nishimura

### 2:05 PM - 2:20 PM

**[S6-19-CL]** Effects of doping of rare earth elements on activity of SrTiO<sub>3</sub>-based photocatalysts for overall water splitting

\*Shigeru Ikeda<sup>1</sup>, Riku Okamoto<sup>1</sup>, Ryota Tomizawa<sup>2</sup>, Taizo Masuda<sup>2</sup>, Koichiro Nakatani<sup>2</sup> (1. Konan Univ. (Japan), 2. TOYOTA MOTOR CORPORATION (Japan))

Chair : Yu Sun and Yoshinobu Nishimura

### 2:20 PM - 2:35 PM

**[S6-20-CL]** Photoaerobic Oxidative *N*-Allylation of Azoles Enabled by Selenium- $\pi$ -Acid Catalysis

\*Theresa Appleson<sup>1</sup>, Tao Lei<sup>1</sup>, Alexander Breder<sup>1</sup> (1. Univ. of Regensburg (Germany))

## ROOM D

Chair : Miho Hatanaka

### 1:45 PM - 2:00 PM

**[S8-06-CL]** "In-silico" Modelling of Fluorescence

\*Daniel Escudero<sup>1</sup> (1. KU Leuven (Belgium))

Chair : Miho Hatanaka

### 2:00 PM - 2:20 PM

**[S8-07-IL]** Valence configuration interaction analysis for excitation properties of open-shell singlet molecules and molecular aggregates

\*Ryohei Kishi<sup>1,2,3,4</sup>, Yasutaka Kitagawa<sup>1,2,3,4,5</sup> (1. Graduate School of Engineering Science, Osaka Univ. (Japan), 2. QIQB, Osaka Univ. (Japan), 3. ICS-OTRI, Osaka Univ. (Japan), 4. RCSEC, Osaka Univ. (Japan), 5. SRN-OTRI, Osaka Univ. (Japan))

Chair : Ryohei Kishi

### 2:20 PM - 2:40 PM

**[S8-08-IL]** On-the-fly molecular dynamics and reduced dimensionality analysis of excited-state branching reactions of stilbene derivatives

\*Tetsuya Taketsugu<sup>1</sup> (1. Hokkaido Univ. (Japan))

# JULY 28 FRI

## ROOM A

Chair : Vincent Chi-Chiu Ko and  
Yasuchika Hasegawa

### 2:35 PM - 2:50 PM

**[S9-21-CL]** Photothermally driven natural vibration of molecular crystal actuators

\*Yuki Hagiwara<sup>1</sup>, Shodai Hasebe<sup>1</sup>, Hiroki Fujisawa<sup>2</sup>, Junko Morikawa<sup>2</sup>, Toru Asahi<sup>1</sup>, Hideko Koshima<sup>1</sup> (1. Waseda Univ. (Japan), 2. Tokyo Institute of Technology (Japan))

Chair : Vincent Chi-Chiu Ko and  
Yasuchika Hasegawa

### 2:50 PM - 3:05 PM

**[S9-22-CL]** Microprinting of hemispherical droplet laser array with optical vortex laser-induced forward transfer

\*Ken-ichi Yuyama<sup>1</sup>, Haruki Kawaguchi<sup>2</sup>, Rong Wei<sup>2</sup>, Takashige Omatsu<sup>2</sup> (1. Osaka Metropolitan Univ. (Japan), 2. Chiba Univ. (Japan))

## ROOM B

Chair : Shigeyuki Masaoka and Wei-Yin Sun

### 2:35 PM - 2:50 PM

**[S5-27-CL]** Development of Function-Integrated Catalytic Systems for Photochemical CO<sub>2</sub> Reduction

\*Mio Kondo<sup>1,2</sup> (1. Graduate School of Engineering, Osaka Univ. (Japan), 2. JST PRESTO (Japan))

Chair : Shigeyuki Masaoka and Wei-Yin Sun

### 2:50 PM - 3:05 PM

**[S5-28-CL]** Redox-mediated Z-scheme water splitting utilizing CuLi<sub>1/3</sub>Ti<sub>2/3</sub>O<sub>2</sub> as H<sub>2</sub>-evolving photocatalyst

\*Hideki Kato<sup>1</sup>, Tanya Kurutach<sup>1</sup>, Qingshan Liu<sup>1</sup>, Toshiki Yamanaka<sup>1</sup>, Shunya Yoshino<sup>1</sup>, Makoto Kobayashi<sup>2</sup> (1. Tohoku Univ. (Japan), 2. Nagoya Univ. (Japan))

### 3:05 PM - 3:20 PM

**[S5-29-CL]** Cancelled

Chair : Shigeyuki Masaoka and Wei-Yin Sun

### 3:20 PM - 3:35 PM

**[S5-30-CL]** Photochemical Conversion of Biogas to Liquid Bioenergy with Chlorine Dioxide

\*Kei Ohkubo<sup>1</sup> (1. Osaka Univ. (Japan))

## ROOM C

Chair : Yu Sun and Yoshinobu Nishimura

### 2:35 PM - 2:50 PM

**[S6-21-CL]** Elucidation of carrier dynamics in visible light absorbing photocatalyst for overall water splitting by transient absorption spectroscopy

\*Ryota Shoji<sup>1</sup>, Vikas Nandal<sup>1</sup>, Hiroyuki Matsuzaki<sup>1</sup>, Kazuhiko Seki<sup>1</sup>, Hiroaki Yoshida<sup>2</sup>, Lishua Lin<sup>3</sup>, Pan Zhenhua<sup>3</sup>, Aihiro Furube<sup>4</sup>, Takashi Hisatomi<sup>3</sup>, Kazunari Domen<sup>3,5</sup> (1. Tsukuba AIST (Japan), 2. Mitsubishi Chemical Corp. (Japan), 3. Shinshu Univ. (Japan), 4. Tokushima Univ. (Japan), 5. Office of Univ. professors., Tokyo Univ. (Japan))

Chair : Yu Sun and Yoshinobu Nishimura

### 2:50 PM - 3:05 PM

**[S6-22-CL]** Triplet-triplet annihilation up-conversion sensitizes metal oxide nanoparticles for photocatalytic reactions

\*Sandra Patricia Gonzalez Lopez<sup>1,2</sup>, Julien Gorenflot<sup>1,2</sup>, Patrick Murton<sup>3</sup>, Maximilian Moser<sup>3</sup>, Iain McCulloch<sup>3</sup>, Frédéric Laquai<sup>1,2</sup> (1. King Abdullah Univ. of Science and Technology (KAUST) (Saudi Arabia), 2. KAUST Solar Center (KSC) (Saudi Arabia), 3. Univ. of Oxford (UK))

### 3:05 PM - 3:20 PM

**[S6-23-CL]** Cancelled

Chair : Yu Sun and Yoshinobu Nishimura

### 3:20 PM - 3:35 PM

**[S6-24-CL]** Mechanistic insights to the photocatalytic reduction of CO<sub>2</sub> in humid vapor phase on Pt/TiO<sub>2</sub>: an *operando* FTIR study

\*Joudy Dankar<sup>1,2</sup>, Céline Pagis<sup>1</sup>, Mickael Rivallan<sup>1</sup>, Mohamad El Roz<sup>2</sup> (1. IFPEN (France), 2. LCS (France))

## ROOM D

Chair : Ryohei Kishi

### 2:40 PM - 2:55 PM

**[S8-09-CL]** A global prediction of the Kataura plot for chiral carbon nanotubes: Topological family effect revealed in the natural helical crystal lattice scheme

Chi-You Liu<sup>1</sup>, Jung-Yin Hsiao<sup>1</sup>, \*Elise Yu-Tzu Li<sup>1</sup> (1. National Taiwan Normal Univ. (Taiwan))

Chair : Ryohei Kishi

### 2:55 PM - 3:15 PM

**[S8-10-IL]** Phosphorescent Intensity of Cyclometalated Iridium(III) Complexes: A Combined DFT and Machine Learning Approach

\*Miho Hatanaka<sup>1</sup> (1. Keio Univ. (Japan))