

## Monday, November 17

**Room: Orbit Hall (B1F)**

8:40-8:55                      **Opening Remarks**

**Room: Orbit Hall (B1F)**                      **8:55-9:50**

**Plenary Lecture**

Chair: Yoshitada Morikawa

---

8:55-9:50              PL1              **A predictive theory of transition metal heterogeneous catalysis**

Jens K. Nørskov

*Stanford University*

---

9:50-10:10                      Coffee break

**Room: Seiuin 1 (2F)**                      **10:10-12:35**

**Session 1 Theoretical and Experimental Elucidation of Interface Reactions**

Chair: Yoshitada Morikawa

---

10:10-10:50              KL1              **Water splitting on some oxynitride and oxysulfide photocatalysts**

Kazunari Domen

*School of Engineering, The University of Tokyo*

10:50-11:20              IL1              **Structure sensitivity of electrocatalytic reactions**

Marc T. M. Koper

*Leiden University*

---

Chair: Yuji Hamamoto

---

11:20-11:40              OP1-1              **Hydrogen Production from Energy Storage Materials using Metal Alloy Catalysts**

Kohsuke Mori

*Graduate School of Engineering, Osaka University*

11:40-12:00              OP1-2              **First-Principles Molecular Dynamics of Water Dissociation and Adsorption of Hydroxyl Groups in Water-bilayer on Pt(322) Stepped Surface**

Hidetoshi Kizaki

*Graduate School of Engineering, Osaka University*

12:00-12:35                      **Poster Short Talk (PP-01 – PP-19)**

---

**Room: Seium 2 (2F)      10:10-12:35**  
**Session 2 Function of Multi-metal Complexes**

Chair: Kazushi Mashima

---

10:10-10:50      KL2      **New Protocols for the Synthesis of Rare-Earth Metal-Ligand Clusters**

Reiner Anwander

*Eberhard Karls Universität Tübingen*

10:50-11:10      OP2-1      **Hydrodehalogenation Reaction of Haloalkanes Catalyzed by Mixed-ligated Paddlewheel Dimolybdenum Complexes**

Hayato Tsurugi

*Graduate School of Engineering Science, Osaka University*

11:10-11:30      OP2-2      **Practical Synthesis of  $[(\eta^6\text{-arene})\text{Ni}(\text{N-heterocyclic carbene})]$  Complexes: Versatile Precursors for Organonickel Chemistry**

Yoichi Hoshimoto

*Graduate School of Engineering, Osaka University*

---

Chair: Hayato Tsurugi

---

11:30-12:00      IL2      **Functionalization of Catalyst Surfaces with Metal Complexes**

Mizuki Tada

*Research Center for Materials Science, Nagoya University*

12:00-12:35      **Poster Short Talk (PC-01 – PC-25)**

---

12:35-14:00      **Lunch Break/Poster Session**

**Room: Orbit Hall (B1F)      14:00-14:55**

**Plenary Lecture**

Chair: Kazushi Mashima

---

14:00-14:55      PL2      **Functional Nanomaterials via Living Crystallization-Driven Self-Assembly**

Ian Manners

*University of Bristol*

---

---

14:55-15:15                      Coffee break

**Room: Seium 1 (2F)                      15:15-17:20**  
**Session 3 Material Design and Realization on Green Energy**

Chair: Hiroshi Katayama-Yoshida

---

15:15-15:55      KL3      **The Role of Spin-Orbit Interaction and Spin-Disorder in Green-IT**

Stefan Blügel

*Forschungszentrum Jülich and JARA*

15:55-16:25      IL3      **Current Status and Future Prospects of Kesterite Photovoltaics**

David B. Mitzi

*Duke University*

Chair: Hidetoshi Kizaki

---

16:25-16:45      OP3-1      **Cu<sub>2</sub>SnZnS<sub>4</sub>-based Solar Cells Fabricated by an Electrochemical Technique**

Shigeru Ikeda

*Research Center for Solar Energy Chemistry, Osaka University*

16:45-17:05      OP3-2      **Theoretical Study of Transition Metal-doped Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> by Screened Korringa-Kohn-Rostoker Green's Function Method**

Tetsuya Fukushima

*Graduate School of Engineering Science, Osaka University*

Chair: Shuto Yamasaka

---

17:05-17:20      ST1      **Ab initio investigations of defect and phase stabilities for thermoelectric pseudo-binary alloy TAGS**

Hikari Shinya

*Graduate School of Engineering Science, Osaka University*

**Room: Seium 2 (2F)                      15:15-17:20**  
**Session 4 Interfacial Chemistry for Novel Functions**

Chair: Ken-ichi Fukui

---

15:15-15:55      KL4      **Surface and Interface Properties of Ionic Liquids**

Hans-Peter Steinrück

*Universität Erlangen-Nürnberg*

15:55-16:25      IL4      **Photofunctional Materials Based on Metal Nanoparticles**

Tetsu Tatsuma

*Institute of Industrial Science, The University of Tokyo*

---

Chair: Tetsuya Tsuda		
16:25-16:45	OP4-1	<b>Design of Core-Shell Nanocomposite Silver Catalyst for Highly Chemoselective Hydrogenations</b> Takato Mitsudome <i>Graduate School of Engineering Science, Osaka University</i>
16:45-17:05	OP4-2	<b>Structural Investigations of Electric Double Layer Transistors: Relation between Microscopic Structures and Device Performances</b> Yasuyuki Yokota <i>Graduate School of Engineering Science, Osaka University</i>
Chair: Kotaro Fukuda		
17:05-17:20	ST2	<b>Photothermal response of gold nanoparticles: single and ensemble particle measurements</b> Kenji Setoura <i>Graduate School of Engineering Science, Osaka University</i>
<b>Room: Orbit Hall (B1F)      17:30-18:30</b>		
<b>Special Lecture</b>		
Chair: Tsuyoshi Kimura		
17:30-18:30	SL	<b>Developments of Nitride-based LEDs and Laser Diodes</b> Shuji Nakamura <i>University of California, Santa Barbara</i>

## Tuesday, November 18

**Room: Orbit Hall (B1F) 8:55-9:50**

**Plenary Lecture**

Chair: Tsuyoshi Kimura

---

8:55-9:50	PL3	<b>Evolutional Science and Engineering of Correlated-Electrons Matter</b> Yoshio Kitaoka <i>Graduate School of Engineering Science, Osaka University</i>
-----------	-----	--

---

9:50-10:10 Coffee break

**Room: Seiun 1 (2F) 10:10-12:15**

**Session 5 Controlling Quantum Effects in Solid**

Chair: Kensuke Kobayashi

---

10:10-10:50	KL5	<b>Imaging integer and fractional quantum Hall edge states</b> Klaus Ensslin <i>ETH Zürich</i>
-------------	-----	--

10:50-11:20	IL5	<b>Slicing a Kondo lattice: the quest for exotic superconductivity in artificially engineered Ce-based superlattices</b> Yuji Matsuda <i>Kyoto University</i>
-------------	-----	---

---

Chair: Hidetomo Usui

---

11:20-11:40	OP5-1	<b>Single spin, photon, and charge manipulation of NV center in diamond</b> Norikazu Mizuochi <i>Graduate School of Engineering Science, Osaka University</i>
-------------	-------	---

11:40-12:00	OP5-2	<b>Shot noise induced by nonequilibrium spin accumulation</b> Tomonori Arakawa <i>Graduate School of Science, Osaka University</i>
-------------	-------	--

---

Chair: Genki Yamashita

---

12:00-12:15	ST3	<b>Pressure-induced Magnetoelectric Transition and Giant Magnetoelectric Effect in Multiferroic <math>RMnO_3</math> (<math>R=Gd, Tb, \text{ and } Dy</math>)</b> Takuya Aoyama <i>Graduate School of Engineering Science, Osaka University</i>
-------------	-----	--

**Room: Seiun 2 (2F)      10:10-12:15**

**Session 6 Organic material Science**

Chair: Takashi Kubo

---

10:10-10:50      KL6      **Chemical Functionalization of Synthetic Carbon Allotropes**  
Andreas Hirsch  
*University of Erlangen-Nuremberg*

10:50-11:20      IL6      **Bent-Shaped Organic Semiconductors for Printed and Flexible Electronics**  
Toshihiro Okamoto  
*School of Frontier Sciences, The University of Tokyo*

---

Chair: Takamitsu Fukuda

---

11:20-11:40      OP6-1      **Porous Molecular Network on Graphenes Formed by Self-Assembly of Dehydrobenzo[12]annulene Derivative**  
Kazukuni Tahara  
*Graduate School of Engineering Science, Osaka University*

11:40-12:00      OP6-2      **Design and Synthesis of Proton-Electron Transfer Complex between Phenols and Phenoxy Radicals**  
Yasukazu Hirao  
*Graduate School of Science, Osaka University*

---

Chair: Haruka Nishiyama

---

12:00-12:15      ST4      **Synthesis and Properties of Oligothiophene-based Cages for Creation of Three-dimensional  $\pi$ -Conjugated Compounds**  
Kazuhiko Adachi  
*Graduate School of Science, Osaka University*

---

12:15-14:40      **Lunch Break/Poster Session**

**Room: Orbit Hall (B1F)      14:40-15:35**

**Plenary Lecture**

Chair: Yoshito Tobe

---

14:40-15:35      PL4      **Synthetic Two-Dimensional Polymers**  
A. Dieter Schlüter  
*ETH Zürich*

---

---

15:35-15:55                      Coffee break

**Room: Seium 1 (2F)                      15:55-18:00**

**Session 7 Energy Harvesting and Saving**

Chair: Akira Sekiyama

---

15:55-16:35              KL7              **Current Status and Future Prospects of Thin-Film Solar Cells**  
Akira Yamada  
*Graduate School of Science and Engineering, Tokyo Institute of Technology*

16:35-17:05              IL7              **Europium-doped Gallium Nitride and Its Application to Environmentally-Friendly Red Light-Emitters**  
Yasufumi Fujiwara  
*Graduate School of Engineering, Osaka University*

---

Chair: Atsushi Koizumi

---

17:05-17:25              OP7-1              **Low Power Operation of Metal-Insulator Transition in Oxide Nano-Structures**  
Teruo Kanki  
*The Institute of Scientific and Industrial Research, Osaka University*

17:25-17:45              OP7-2              **Recent Development in Nanostructured Thermoelectric Materials**  
Yuji Ohishi  
*Graduate School of Engineering, Osaka University*

---

Chair: Hikari Shinya

---

17:45-18:00              ST5              **Fabrication of Ultrahigh Density Ge Nanodots as Phonon Scatterers in Si Films and Their Thermoelectric Properties**  
Shuto Yamasaka  
*Graduate School of Engineering Science, Osaka University*

**Room: Seium 2 (2F)                      15:55-18:00**

**Session 8 Organic material Science**

Chair: Satoshi Minakata

---

15:55-16:35              KL8              **Organophosphorus Avenues toward Self-Assembled Nanomaterials**  
Thomas Baumgartner  
*University of Calgary*

16:35-17:05	IL8	<b>Materials for Organic Electronics Using Quasiplanar Structure as a Key Scaffold</b> Atsushi Wakamiya <i>Institute for Chemical Research, Kyoto University</i> <hr/> Chair: Yutaka Ie
17:05-17:25	OP8-1	<b>Crystalline Supramolecular Nanofibers Composed of Noncentrosymmetric <math>\pi</math>-Conjugated Molecules</b> Ichiro Hisaki <i>Graduate School of Engineering, Osaka University</i>
17:25-17:45	OP8-2	<b>Synthesis and Physicochemical Properties of Phosphorus Analogues of Pyromellitic Diimides as Novel Electron-acceptors</b> Youhei Takeda <i>Graduate School of Engineering, Osaka University</i> <hr/> Chair: Kazuhiko Adachi
17:45-18:00	ST6	<b>Catalytic Radical Reaction Catalyzed by Niobium and Tantalum Complexes bearing <math>\alpha</math>-Diimine Ligands</b> Haruka Nishiyama <i>Graduate School of Engineering Science, Osaka University</i>
18:30~20:30		<b>Banquet (VERDE B1F)</b>

---



## Wednesday, November 19

Room: Orbit Hall (B1F) 8:55-9:50

### Plenary Lecture

Chair: Hiroshi Katayama-Yoshida

---

8:55-9:55 PL5 **Spintronics Materials and Devices for Nonvolatile VLSIs**  
Hideo Ohno  
*Tohoku University*

9:50-10:10 Coffee break

Room: Seiun 1 (2F) 10:10-12:15

### Session 9 Novel Development of Nanophotonics

Chair: Masaaki Ashida

---

10:10-10:50 KL9 **Laser Trapping Assembling Dynamics of Molecules and Nanoparticles**  
Hiroshi Masuhara  
*National Chiao Tung University*

10:50-11:20 IL9 **Plasmonic Optical Tweezers toward Chemical Applications**  
Yasuyuki Tsuboi  
*Graduate School of Science, Osaka City University*

Chair: Yutaka Nagasawa

---

11:20-11:40 OP9-1 **Optical Trapping of Nanomaterials**  
Yosuke Minowa  
*Graduate School of Engineering Science, Osaka University*

11:40-12:00 OP9-2 **Selective Assembly Microstructures of Uniforms Silver Nanoparticles by Using Radiation Pressure of CW lasers**  
Syoji Ito  
*Graduate School of Engineering Science, Osaka University*

Chair: Takuya Aoyama

---

12:00-12:15 ST7 **UV-excited carrier multiplication in bulk Si crystals investigated by terahertz spectroscopy**  
Genki Yamashita  
*Graduate School of Engineering Science, Osaka University*

**Room: Seiu 2 (2F) 10:10-12:15**

**Session 10 Theoretical Aspects of Functional Materials**

Chair: Mitsutaka Okumura

---

10:10-10:50 KL10 **Unraveling Nanoparticle Properties using Theoretical Methods**

Christine M. Aikens  
*Kansas State University*

10:50-11:20 IL10 **Toward Controlling Complex Chemical Reactions in the "Molecular Aggregation States" -From Multiscale Simulation to Computational Molecular Technology-**

Masataka Nagaoka  
*Graduate School of Information Science, Nagoya University*

Chair: Ryohei Kishi

---

11:20-11:40 OP10-1 **Geometric and Electronic Structures of TbPc<sub>2</sub> Complex: A Density Functional Theory Study**

Yasutaka Kitagawa  
*Graduate School of Engineering Science, Osaka University*

11:40-12:00 OP10-2 **QM-only and QM/MM Studies of Electronic Structure and Dioxygen Binding in Hemocyanin**

Toru Saito  
*Graduate School of Science, Osaka University*

Chair: Kenji Setoura

---

12:00-12:15 ST8 **Synergy Effect of the Donor- $\pi$ -Donor Nature and the Intermediate Diradical Character on the Second Hyperpolarizabilities**

Kotaro Fukuda  
*Graduate School of Engineering Science, Osaka University*

**Room: Seiu 1 (2F)**

12:15-12:30 **Closing Remarks**

---