# ACTIVITIES OF JOINT USAGE/RESEARCH CENTER

## **JURC Cooperative Research Subjects 2017**

 $(1 \text{ April } 2017 \sim 31 \text{ March } 2018)$ 

## STARTING-UP SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY JURC)

Synthesis of Transition Metal Complexes with a Pincer-Type Phosphaalkene Ligand and Their Application to Catalytic Reactions MATSUO, Tsukasa, Faculty of Science and Engineering / Graduate School of Science and Engineering Research, Kindai University Host in JURC TAKEUCHI, Katsuhiko

Feasibility Study of Novel Cooling Devices with Perovskite Semiconductors

YAMADA, Noboru, Department of science of technology Innovation, Nagaoka University of Technology

Host in JURC KANEMITSU, Yoshihiko

Investigation of Carrier Transport Mechanism in Halide-perovskitebased Photodevices

YAMADA, Yasuhiro, Department of Physics, Graduate School of Science, Chiba University

Host in JURC KANEMITSU, Yoshihiko

Many Body Interactions between Excitons in Semiconductor

OGAWA, Yoshihiro, Joetsu University of Education

Host in JURC KANEMITSU, Yoshihiko

Investigation on Quantum Properties of Luminescent Nanomaterials Using Novel Techniques of Laser Microscopic Spectroscopy IHARA, Toshiyuki, Advanced ICT Research Institute, National Institute of Information and Communications Technology

Host in JURC KANEMITSU, Yoshihiko

Iron-Catalyzed Enantioselective C-C Bond Formation ILIES, Laurean, Department of Chemistry, School of Science, The University of Tokyo

Host in JURC NAKAMURA, Masaharu

Study on First-raw Late Transition-metal Complexes Bearing Anionic Tridentate Ligand

YAMAGUCHI, Yoshitaka, Faculty of Engineering, Division of Materials Science and Chemical Engineering, Yokohama National University

Host in JURC NAKAMURA, Masaharu

Analysis of Complex Networks with Degree Correlations TAKEMOTO, Kazuhiro, Department of Bioscience and Bioinformatics, Kyushu Institute of Technology

Host in JURC AKUTSU, Tatsuya

Control and Analysis of Complex Networks via Minimum Dominating Sets

JOSE, C. Nacher, Department of Information Science, Faculty of Science, Toho University

Host in JURC AKUTSU, Tatsuya

Genome Analysis of New Giant DNA Virus Isolated from Hot Spring Water in Japan

TAKEMURA, Masaharu, Faculty of Science, Tokyo University of Science

Host in JURC OGATA, Hiroyuki

I : International Joint Research

F: Female PI

Establishment of a New Virus-evolution-hypothesis Through an Intensive Quest of Megaviruses in a Highly Enclosed Inlet, Uranouchi Bay, Where Various Algal Blooms Frequently Occur NAGASAKI, Keizo, Faculty of Agriculture and Marine Science, Kochi University

Host in JURC OGATA, Hiroyuki

New Prediction Method for Metabolic Pathway from Genome and Metagenome by Combination of MAPLE and GENIES TAKAMI, Hideto, Research and Development Center for Sub-

marine Resources, Japan Agency for Marine-Earth Science and Technology

Host in JURC OGATA, Hiroyuki

Machine Learning Based on Sparsity Regularization with Auxiliary Genomic Information

SHIGA, Motoki, Informatics Course, Department of Electrical, Electronic and Computer Engineering, Faculty of Engineering, Gifu University

Host in JURC MAMITSUKA, Hiroshi Ι

Creation of Highly Active Polypodna Complexes and Their Intra-

NISHIKAWA, Makiya, Faculty of Pharmaceutical Sciences, Tokyo University of Science

Host in JURC FUTAKI, Shiroh

Development of Novel Heteroazulene Oligomer Toward Organic Functional Dves

KUROTOBI, Kei, National Institute of Technology, Kurume Col-

Host in JURC MURATA, Yasujiro

Synthesis of  $\pi$ -Extended Thienofuran Derivatives by Dehydrative Cyclization, and Their Properties

SUGA, Seiji, Graduate School of Natural Science and Technology, Okayama University

Host in JURC MURATA, Yasujiro

Synthesis of Metal Complexes with Three-dimensional  $\pi$ -Systems and their Performance as Organic Semiconductors

MURATA, Michihisa, Department of Applied Chemistry, Osaka Institute of Technology

Host in JURC MURATA, Yasujiro

Molecular Engineering of Highly Crystalline Organic Semiconductors via Precursor Approaches

SUZUKI, Mitsuharu, Graduate School of Materials Science, Nara Institute of Science and Technology (NAIST)

Host in JURC MURATA, Yasujiro

Study on Highly Efficient Transportation of Metal Ions through a Membrane Containing Ionic Liquid

MUKAI, Hiroshi, Faculty of Education, Kyoto University of Education

Host in JURC SOHRIN, Yoshiki

Elucidation of Hydrogen Distribution in Single-crystalline Pd Nanoparticles

YAMAUCHI, Miho, International Institute for Carbon-Neutral Energy Research, Kyushu University

Host in JURC TERANISHI, Toshiharu

Design and Creation of New Functional Material Having Both Optical Diagnostic and Therapeutic Effects using Metal Nanoparticle

ISHIHARA, Miya, National Defense Medical College **Host in JURC** TERANISHI, Toshiharu

Test of Resonant Effect in Plasmon Heating of Periodic Lattice of Metal Domain

SHIMADA, Ryoko, Department of Mathematical and Physical Sciences, Faculty of Science, Japan Women's University

Host in JURC WATANABE, Ĥiroshi

Fabrication and Evaluation of Dye-sensitized Solar Cells using Flavonoid Compounds, and Their Theoretical Studies Toward Improvement of the Efficiency

YOSHIDA, Kumi, Department of Complex Systems Science, Graduate School of Information Science, Nagoya University

Host in JURC MURATA, Yasujiro; WAKAMIYA, Atsushi

Structure Analysis of Monolayer Assembly with  $\pi$ -Conjugated Units Studied by pMAIRS

YAMAMOTO, Shunsuke, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University

Host in JURC HASEGAWA, Takeshi

# EXPANDING SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY JURC)

Fundamental Study on Micro-fabrication of Metal with Controlling Laser Absorption

KUSABA, Mitsuhiro, Electronics, Information and Communication Engineering, Osaka Sangyo University

Host in JURC HASHIDA, Masaki

Advanced Functionality on Materials Induced by Intense THz Interaction

NAGASHIMA, Takeshi, Faculty of Science and Engineering, Setsunan University

Host in JURC HASHIDA, Masaki

A Study of Laser Driven High-intensity Terahertz Surface Wave TOKITA, Shigeki, Institute of Laser Engineering, Osaka University **Host in JURC** SAKABE, Shuji

Diagnostics of Li-Ion Batteries with Laser-Accelerated Protons KATO, Yoshiaki, The Graduate School for the Creation of New Photonics Industries

Host in JURC SAKABE, Shuji

Development on a Repetitive Laser-driven Neutron Source ARIKAWA, Yasunobu, Institute of Laser Engineering, Osaka University

Host in JURC INOUE, Shunsuke

Proposal of a CEP-stabilized Free-Electron Laser and Fabrication of a Superconducting Electron Accelerating Cavity Operated by Small Electricity Power

HAJIMA, Ryoichi, National Institutes for Quantum and Radiological Science and Technology, Quantum Beam Science Research Division

Host in JURC IWASHITA, Yoshihisa

Study on Magnification of the Pulsed-neutron Transmission Image Using the Sextupole Magnet, Aimed at Visualization of Charge and Discharge in the Electrode Materials of Li-ion Batteries KINO, Koichi, Research Institute for Measurement and Analytical Instrumentation, National Institute of Advanced Industrial Science and Technology

Host in JURC IWASHITA, Yoshihisa

Research and Development on Future Accelerator Toward ILC Project

HAYANO, Hitoshi, Accelerator Laboratory, High Energy Accelerator Research Organization

Host in JURC IWASHITA, Yoshihisa

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Research on the High-performance Superconducting Cavity with the Inner-surface Preparation

by Nitrogen-doping and Thin-film Creation Processes

SAEKI, Takayuki, Accelerator Laboratory, High Energy Accelerator Research Organization

Host in JURC IWASHITA, Yoshihisa

X-Ray Structural Studies on Reaction Mechanism of Maleylacetate Reductase

OIKAWA, Tadao, Faculty of Chemistry, Materials and Bioengineering, Kansai University

Host in JURC FUJII, Tomomi

X-ray Crystallographic Studies on Thermostability and Substrate Specificity of L-Asparaginase

KATO, Shiro, International Institute of Rare Sugar Research and Education, Kagawa University

Host in JURC FUJII, Tomomi

Activation of Small Molecules at the Reaction Sites Composed of Transition-metal and Heavier Typical Elements

OKAZAKI, Masaaki, Graduate School of Science and Technology, Hirosaki University

Host in JURC OZAWA, Fumiyuki

Development of Iron Polycarboxylate Complexes which Catalyze Oxidation Reactions

SUGIURA, Masaharu, Faculty of Life Sciences, Kumamoto University

Host in JURC NAKAMURA, Masaharu

Elucidation of Electronic Structures of Cycloparaphenylenes and Their Application to Materials Science

UCHIYAMA, Masanobu, Graduate School of Phamaceutical Science, The University of Tokyo

Host in JURC YAMAGO, Shigeru

Efficient Molecular Network Analysis through Statistical Machine Learning

KAYANO, Mitsunori, Research Center for Global Agromedicine, Obihiro University of Agriculture and Veterinary Medicine Host in JURC MAMITSUKA, Hiroshi

Cell Penetrating Peptide-based Intracellular Delivery of Inhibitors of Protein-protein Interactions

OHKANDA, Junko, Academic Assembly School of Science and Technology Institute of Agriculture, Shinsyu University

Host in JURC FUTAKI, Shiroh

A Study of Reactivity on Open-shell Molecules in Macrocyclic Systems

ABE, Manabu, Graduate School of Science, Hiroshima University **Host in JURC** YAMAGO, Shigeru

Excited-state Dynamics of Cycloparaphenylene Dications MAJIMA, Tetsuro, The Institute of Scientific and Industrial Research, Osaka University

Host in JURC YAMAGO, Shigeru

Host-guest Chemistry of Cycloparaphenylenes and Fullerene Derivatives

MATSUO, Yutaka, School of Chemistry and Materials Science, University of Science and Technology of China

Host in JURC YAMAGO, Shigeru

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Exploration of Non-lead Perovskite Solar Cell and Development of Novel Efficient Organic Hole Transfer Layer

SAEKI, Akinori, Graduate School of Engineering, Osaka University **Host in JURC** WAKAMIYA, Atsushi

Organic Photovoltaic Devices Composed of Novel Organic Semiconductors

IE, Yutaka, The Institute of Scientific and Industrial Research, Osaka University

Host in JURC MURATA, Yasujiro

Flux Study of Bioactive Trace Metals in the East China Sea NAKAGUCHI, Yuzuru, Faculty of Science and Engineering, Kindai University

Host in JURC SOHRIN, Yoshiki

Structural Analyses for Adhesive Mechanism in Tri-block Polymer Thin Films Using Neutron Reflectivity and Grazing Incidence X-ray Scattering Measurement

MIYAZAKI, Tsukasa, Comprehensive Research Organization for Science and Society

Host in JURC TAKENAKA, Mikihito

Dynamics of Guest Chains in Polymer Networks with Different Crosslinking Types

KATASHIMA, Takuya, Graduate School of Science, Osaka University

Host in JURC MATSUMIYA, Yumi

Dynamical Correlations between Molecules in Polymeric Liquids SUKUMARAN, Sathish Kumar, Graduate School of Organic Materials Science, Yamagata University

Host in JURC WATANABE, Hiroshi

# STARTING-UP SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

Study on the Regulatory Mechanism of Plant Epidermal Cell Differentiation

TOMINAGA, Rumi, Graduate School of Biosphere Science, Hiroshima University

Host in JURC AOYAMA, Takashi

Study on Lipid Secretion Pathways of Plant Cells

YAZAKI, Kazufumi, Research Institute for Sustainable Humanosphere, Kyoto University

Host in JURC AOYAMA, Takashi

Dynamics of the Transcription Factor ARR1 on Plant Chromosomal DNA

KIM, Jong-Myong, RIKEN Center for Sustainable Resource Science

Host in JURC AOYAMA, Takashi

New Cellular Functions of Acyldopamine

ITO, Akihiro, RIKEN Center for Sustainable Resource Science, Chemical Genomics Research Group

Host in JURC UESUGI, Motonari

Study of Spin-filtering Effect of the Magnetic Insulator Films with Perpendicular Magnetic Anisotropy

TANAKA, Masaaki, Department of Physical Science and Engineering, Nagoya Institute of Technology

Host in JURC ONO, Teruo

Electric Field Induced Skyrmion Motion

NAKATANI, Yoshinobu, Department of Communication Engineering and Informatics, The University of Electro-Communications **Host in JURC** ONO, Teruo

Development of Catalysts for Regio- and Stereoselective Oxidation ITO, Akichika, Gifu Pharmaceutical University

Host in JURC KAWABATA, Takeo

Selective Chemical Modification of Biomolecules in Membrane by Functionalized Catalysts

KUNISHIMA, Munetaka, Faculty of Pharmaceutical Sciences, Institute of Medical, Pharmaceutical, and Health Sciences, Kanazawa University

Host in JURC KAWABATA, Takeo

Characteristics of Membrane Vesicles Produced by Intestinal Bacteria and Their Biogenesis

KURATA, Atsushi, Faculty of Agriculture, Kindai University **Host in JURC** KURIHARA, Tatsuo

Structural Control and Functional Development of Alkali Silicate Glasses by High Pressure Synthesis

MASAI, Hirokazu, Department of Materials and Chemistry, National Institute of Advanced Industrial Science and Technology **Host in JURC** SAITO, Takashi

Application of Surfactants for Separation of Boron Group Elements as Synergist

KURAHASHI, Kensuke, Environmental and Materials Chemistry Course, Osaka Prefecture University College of Technology **Host in JURC** SOHRIN, Yoshiki

Development of Organic Reagents Highly Selective for the Extraction and Adsorption of Rare Metals

YAMAZAKI, Shoko, Department of Chemistry, Nara University of Education

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Host in JURC UMETANI, Shigeo

Precise Analyses of Hierarchical Structure of Polymer Composite Materials by Electron/X-ray/Neutron Beams

MURASE, Hiroki, Faculty of Home Economics, Kyoritsu Women's University

Host in JURC TSUJII, Yoshinobu

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Room Temperature Operation of  $Au_{25}$  Cluster Single-electron Transistor

MAJIMA, Yutaka, Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology

Host in JURC TERANISHI, Toshiharu

Dielectric Relaxation of Linear Rouse Chains having Type-A Dipole and Undergoing Head-to-Head Association and Dissociation

KWON, Youngdon, School of Chemical Engineering, Sungkyunkwan University

Host in JURC MATSUMIYA, Yumi

The Sequence Control of Two-component Multiblock Copolymers and the Investigation of Bulk and Surface Properties

TAKANO, Atsushi, Graduate School of Engineering, Nagoya University

Host in JURC WATANABE, Hiroshi

Mode of Action Study of Benzoylphenylurea Insecticides at the Molecular Level

NAKAGAWA, Yoshiaki, Graduate School of Agriculture, Kyoto University

Host in JURC WATANABE, Bunta

Synthesis and Application of Macrocyclic Compounds Incorporating Triphenylamine Units

IWANAGA, Tetsuo, Department of Chemistry, Faculty of Science, Okayama University of Science

Host in JURC MURATA, Yasujiro

Study of Surface Enhanced Infrared Absorption by Using Multipleangle Incidence Resolution Spectrometry

SHIMADA, Toru, Faculty of Education, Hirosaki University **Host in JURC** HASEGAWA, Takeshi

Even-odd Effects on Film Structures of Dicarboxylic Acids on Air/Water Interface and Their Atmospheric Implications HAMA, Tetsuya, Institute of Low Temperature Science, Hokkaido University

Host in JURC HASEGAWA, Takeshi

# EXPANDING SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

Modulation of New Cellular Functions of Vitamin D NAGASAWA, Kazuo, Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology **Host in JURC** UESUGI, Motonari

Developments of Highly Functional Spinel Ferrite Thin Films as a Novel Spintornic Materials

NAGAHAMA, Taro, Laboratory of Advanced Materials Chemistry, Graduate School of Engineering, Hokkaido University

Host in JURC ONO, Teruo

Measurements of Giant Magnetoresistance Effect in Magnetic Nanowires with Multilayer Structure

YAMADA, Keisuke, Faculty of Engineering, Gifu University **Host in JURC** ONO, Teruo

Magnetic Nanostructures Confined or Created by Electric Field CHIBA, Daichi, School of Physical Science and Engineering, Nagoya Institute of Technology

Host in JURC ONO, Teruo

A Study on the Relationship between Structures and Functions for Organic Devices

FUKUSHIMA, Tatsuya, Department of Chemical Science and Engineering, Kobe University

Host in JURC KAJI, Hironori

Theoretical Study on Chemoselective Acylation Catalyzed by 4-Pyrrolidinopyridine Derivatives

YAMANAKA, Masahiro, Department of Chemistry, College of Science, Rikkyo University

Host in JURC KAWABATA, Takeo

Studies on the Function and Formation Mechanism of the Bound D-Amino Acids in Food Proteins

OMORI, Taketo, Faculty of Engineering, Osaka Institute of Technology

Host in JURC KURIHARA, Tatsuo

Functional Study of Metal-induced Membrane Proteins in Microbial Metal Respiration

MIHARA, Hisaaki, Department of Biotechnology, College of Life Sciences, Ritsumeikan University

Host in JURC KURIHARA, Tatsuo

Search for Four Wave-mixing in the Vacuum

HONMA, Kensuke, Graduate School of Science, Hiroshima University

Host in JURC SAKABE, Shuji

Exploration of Electric-field-effect-induced Functional Properties of Transition Metal Oxides

HATANO, Takafumi, Department of Crystalline Materials Science, Nagoya University

Host in JURC KAN, Daisuke

In-situ Measurements of Physical Properties and Crystallization Process of Glasses Under High Temperatures and High Pressures MASUNO, Atsunobu, Graduate School of Science and Technology, Hirosaki University

Host in JURC SHIMAKAWA, Yuichi

Photochemical Control of Gel-gel Transitions in Polymer-brushafforded Silica Particle/Photoresponsive Liquid Crystals

YAMAMOTO, Takahiro, Research Institute for Sustainable Chemistry, National Institute of Advanced Industrial Science and Technology (AIST)

Host in JURC OHNO, Kohji

Synthesis and Characterization of Novel Narrow Band Gap Semiconductor Nanocrystals

TACHIBANA, Yasuhiro, School of Aerospace, Mechanical and Manufacturing Engineering, RMIT University

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Host in JURC TERANISHI, Toshiharu

Identification of Proteins Interacting with Cell-penetrating Peptides for Cancer Targeting

KUWATA, Keiko, Institute of Transformative Bio-Molecules, Nagoya University

Host in JURC FUTAKI, Shiroh

Electrical Control and Detection of Spin of NV Center MAKINO, Toshiharu, Energy Technology Research Institute, National Institute of Advanced Industrial Science and Technology (AIST)

Host in JURC MIZUOCHI, Norikazu

Toward Long Spin Coherence Time of NV Center at Diamond Surface Region

TOKUDA, Norio, Faculty of Electrical and Computer Engineering, Institute of Science and Engineering, Kanazawa University **Host in JURC** MIZUOCHI, Norikazu

Characterization Toward Ultra-high Sensitivity Sensor by Using Diamond

HATANO, Mutsuko, Tokyo Institute of Technology, School of Engineering, Department of Electrical and Electronic Engineering

Host in JURC MIZUOCHI, Norikazu

Study on the Biosynthetic Pathway of Steroidal Glycoalkaloids in *Solanaceae* Plants

MIZUTANI, Masaharu, Graduate School of Agricultural Science, Kobe University

Host in JURC WATANABE, Bunta

# SUBJECTS FOCUSING OF JOINT USAGE OF JURC/ICR FACILITIES

Elucidation of a Mechanism of Crystalline-to-amorphous Framework Transformation in Coordination Polymers

INUKAI, Munehiro, Faculty of Science and Technology, Tokushima University

Host in JURC KAJI, Hironori

Nano-electron Spectroscopic Study on Hydrogen and Helium Behavior in Plasma Facing Materials for Nuclear Fusion Devices MIYAMOTO, Mitsutaka, Interdisciplinary Faculty of Science and Engineering, Shimane University

Host in JURC KURATA, Hiroki

Fabrication of Helical Ultrathin Au Nanowires with Chiral Photonicmetamaterial Property

KAWAI, Takeshi, Faculty of Engineering, Tokyo University of Science

Host in JURC KURATA, Hiroki

Analysis of Local Magnetic Moment in Nd-Fe-B Magnet by Electron Energy-loss Spectroscopy

SAITO, Hikaru, Interdisciplinary Graduate School of Engineering Sciences, Kyushu University

Host in JURC KURATA, Hiroki

Elucidation of the Fluorous Interactions in the Crystal Structures of Fluorine-containing Conjugated Molecules by the Single-crystal X-ray Structural Analysis

AGOU, Tomohiro, Department of Biomolecular Functional Engineering, College of Engineering, Ibaraki University

Host in JURC TOKITOH, Norihiro

Synthesis and Elucidation of Properties of Unsymmetrically-Substituted Disilyne and Related  $\pi$ -Electron Systems

IWAMOTO, Takeaki, Graduate School of Science, Tohoku University

Host in JURC TOKITOH, Norihiro

Synthesis and Structural Elucidation of Unsaturated Compounds of Germanium

MATSUO, Tsukasa, Faculty of Science and Engineering, Kindai University

Host in JURC TOKITOH, Norihiro

Experimental Electron Density Distribution Analysis of Organosilicon Compounds

HASHIZUME, Daisuke, Center for Emergent Matter Science, RIKEN

Host in JURC TOKITOH, Norihiro

Synthesis and Emission Properties of Aromatic Compounds Containing a Phosphorus Atom

NAGAHORA, Noriyoshi, Department of Chemistry, Faculty of Science, Fukuoka University

Host in JURC TOKITOH, Norihiro

Synthesis and Structure of Kinetically Stabilized Main Group Element Compounds using 9-Triptycylmethyl Groups MINOURA, Mao, Faculty of Science, Rikkyo University Host in JURC TOKITOH, Norihiro Study of the Mechanism of Steroid Hormone Production Using Imaging Mass Spectrometry and Targeted Proteomics

HATANO, Osamu, Department of Anatomy and Cell Biology, Nara Medical University

Host in JURC ISOZAKI, Katsuhiro

Isolation and Mass Spectrometry of Intermediate Clusters Synthesized by Ligand Exchange Reaction

NEGISHI, Yuichi, Faculty of Science, Department of Applied Chemistry, Tokyo University of Science

Host in JURC ISOZAKI, Katsuhiro

#### SUBJECTS ENCOURAGING JOINT PROGRAM

Exploring for Novel Functional Transition-metal Oxides by High-pressure Synthesis

CHEN, Wei-Tin, Center for Condensed Matter Sciences, National Taiwan University

Host in JURC SHIMAKAWA, Yuichi

Elucidating the Cycle of Dissolved and Particulate Trace Metals in the Ocean Based on Stable Isotope Analysis

HO, Tung-Yuan, Research Center for Environmental Changes, Academia Sinica

Host in JURC TAKANO, Shotaro

Precise Synthesis of Photo-functional Polymers Using Organocatalyzed Living Radical Polymerization

GOTO, Atsushi, School of Physical and Mathematical Sciences, Nanyang Technological University

Host in JURC TSUJII, Yoshinobu

Novel Drug-delivery System Using Albumin as a Reservoir SAGAN, Sandrine, Laboratoire des Biomolécules, UMR7203 CNRS—University Pierre et Marie Curie –École Normale Supérieure Paris **Host in JURC** FUTAKI, Shiroh

The Twelfth International Workshop for East Asian Young Rheologists

INOUE, Tadashi, Graduate School of Science, Osaka University **Host in JURC** WATANABE, Hiroshi

## **JURC Publications (Selected Examples)**

(until 31 May 2017)

## A Square-Planar Complex of Platinum(0)

Takeuchi, K.; Taguchi, H.; Tanigawa, I.; Tsujimoto, S.; Matsuo, T.; Tanaka, H.; Yoshizawa, K.; Ozawa, F., *Angew. Chem. Int. Ed.*, **55**, 15347-15350 (2016).

#### Abstract

The Pt<sup>0</sup> complex [Pt(PPh<sub>3</sub>)(Eind<sub>2</sub>-BPEP)] with a pyridine-based PNP-pincer-type phosphaalkene ligand (Eind<sub>2</sub>-BPEP) has a highly planar geometry around Pt with  $\sum$ (Pt)=358.6°. This coordination geometry is very uncommon for formal d<sup>10</sup> complexes, and the Pd and Ni homologues with the same ligands adopt distorted tetrahedral geometries. DFT calculations reveal that both the Pt and Pd complexes are M<sup>0</sup> species with nearly ten valence electrons on the metals whereas their atomic orbital occupancies are evidently different from one another. The Pt complex has a higher occupancy of the atomic 6s orbital because of strong s–d hybridization due to relativistic effects, thereby adopting a highly planar geometry reflecting the shape and orientation of the partially  $d_{x^2-y^2}$  unoccupied orbital.

## Interfacial Charge-Carrier Trapping in CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>-Based Heterolayered Structures Revealed by Time-Resolved Photoluminescence Spectroscopy

Yamada, Y.; Yamada, T.; Shimazaki, A.; Wakamiya, A.; Kanemitsu, Y., *J. Phys. Chem. Lett.*, **7**, 1972-1977 (2016).

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### **Abstract**

The fast-decaying component of photoluminescence (PL) under very weak pulse photoexcitation is dominated by the rapid relaxation of the photoexcited carriers into a small number of carrier-trapping defect states. Here, we report the subnanosecond decay of the PL under excitation weaker than 1 nJ/cm² both in CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>-based heterostructures and bare thin films. The trap-site density at the interface was evaluated on the basis of the fluence-dependent PL decay profiles. It was found that high-density defects determining the PL decay dynamics are formed near the interface between CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> and the hole-transporting Spiro-OMeTAD but not at the CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>/TiO<sub>2</sub> interface and the interior regions of CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> films. This finding can aid the fabrication of high-quality heterointerfaces, which are required improving the photoconversion efficiency of perovskite-based solar cells.

## Critical Controllability in Proteome-wide Protein Interaction Network Integrating Transcriptome

Ishitsuka, M.; Akutsu, T.; Nacher, J. C., Sci. Rep., 6, [23541-1]-[23541-13] (2016).

### Abstract

Recently, the number of essential gene entries has considerably increased. However, little is known about the relationships between essential genes and their functional roles in critical network control at both the structural (protein interaction network) and

dynamic (transcriptional) levels, in part because the large size of the network prevents extensive computational analysis. Here, we present an algorithm that identifies the critical control set of nodes by reducing the computational time by 180 times and by expanding the computable network size up to 25 times, from 1,000 to 25,000 nodes. The developed algorithm allows a critical controllability analysis of large integrated systems composed of a transcriptome- and proteome-wide protein interaction network for the first time. The data-driven analysis captures a direct triad association of the structural controllability of genes, lethality and dynamic synchronization of co-expression. We believe that the identified optimized critical network control subsets may be of interest as drug targets; thus, they may be useful for drug design and development.

## Detailed Analysis of Charge Transport in Amorphous Organic Thin Layer by Multiscale Simulation without Any Adjustable Parameters

Uratani, H.; Kubo, S.; Shizu, K.; Suzuki, F.; Fukushima, T.; Kaji, H., *Sci. Rep.*, **6**, 39128, doi: 10.1038/srep39128 (2016). **Abstract** 

Hopping-type charge transport in an amorphous thin layer composed of organic molecules is simulated by the combined use of molecular dynamics, quantum chemical, and Monte Carlo calculations. By explicitly considering the molecular structure and the disordered intermolecular packing, we reasonably reproduce the experimental hole and electron mobilities and their applied electric field dependence (Poole–Frenkel behaviour) without using any adjustable parameters. We find that the distribution of the density-of-states originating from the amorphous nature has a significant impact on both the mobilities and Poole–Frenkel behaviour. Detailed analysis is also provided to reveal the molecular-level origin of the charge transport, including the origin of Poole–Frenkel behaviour.

# Activation of Dihydrogen by Masked Doubly Bonded Aluminum Species

Nagata, K.; Murosaki, T.; Agou, T.; Sasamori, T.; Matsuo, T.; Tokitoh, N., *Angew. Chem. Int. Ed.*, **55**, 12877-12880 (2016). **Abstract** 

Activation of dihydrogen by masked dialumenes (Al=Al doubly bonded species) is reported. Reactions of barrelene-type dialumanes, which have the reactivity as masked equivalents of 1,2-diaryldialumenes ArAl=AlAr, with  $\rm H_2$  afforded dihydroalumanes ArAlH2 at room temperature (Ar: bulky aryl groups). These dihydroalumanes form hydrogen-bridged dimers [ArHAl( $\mu$ -H)]2 in the crystalline state, while a monomer–dimer equilibrium was suggested in solution. The 1,2-diaryldialumenes generated from the barrelene-type dialumanes are the putative active species in the cleavage of  $\rm H_2$ .