

**The 5<sup>th</sup> International Symposium of Quantum Beam Science (ISQBS2020) at Ibaraki University**  
**-Chirality in Material Science: Current Status and Future Prospects-**

**19 November (Thu) 2020**

- 09:30 - 10:00            Opening Remarks  
Hiroyuki Ohta (President of Ibaraki University, Japan)  
Teruyuki Ikeda (Director of Institute of Quantum Beam Science,  
Ibaraki University, Japan)  
Hiroyuki Nishikawa (Chair of Organizing Committee, Ibaraki University, Japan)
- Chair: Hiroyuki Nishikawa
- 10:00 - 10:50            **19-O01 (Plenary Lecture)**  
Helical conjugated polymer: synthesis and optoelectronic properties  
Kazuo Akagi (Ritsumeikan University, Japan)
- 10:50 - 11:15            **19-O02**  
How to design chiral fluorophores aiming at enhanced circularly polarized  
luminescence phenomena  
Ken-ichi Sugiura (Tokyo Metropolitan University, Japan)
- 11:15 - 11:30            Coffee Break
- 11:30 - 11:55            **19-O03**  
Synthesis and evaluation of binaphthiol-based functional molecules  
Kazunori Tsubaki (Kyoto Prefectural University, Japan)
- 11:55 - 12:15            **19-O04**  
Fluorinated Helicenes: Synthesis and Properties  
Tomohiro Agou (Ibaraki University, Japan)
- 12:15 - 13:00            Lunch
- 13:00 - 14:40            **Poster Session 1**
- 14:40 - 15:00            Coffee Break
- Chair: Kazunori Tsubaki
- 15:00 - 15:50            **19-O05 (Plenary Lecture)**  
Chiromorphology as a crossroad of chemistry and biology  
Reiko Kuroda (Chubu University, Japan)

- 15:50 - 16:15            **19-O06**  
Triazole-linked DNA and RNA: from chiral monomers to oligomers and duplexes  
Tomoko Fujino (University of Tokyo, Japan)
- 16:15 - 16:35            **19-O07**  
Tuning of type 1 copper site and stability through the non-covalent weak interaction in  
second coordination sphere of blue copper protein  
Takahide Yamaguchi (Ibaraki University, Japan)
- 16:35 - 17:00            **19-O08**  
Syntheses of natural products via aryl ether formation  
Itaru Sato (Ibaraki University, Japan)
- 17:00 - 17:20            Coffee Break
- 17:20 - 18:10            **19-O09** (*Plenary Lecture*)  
Chiral molecule to chiral functional nanoobjects  
Reiko Oda (Université Bordeaux, France)
- Chair: Ken-ichi Sugiura

**20 November (Fri) 2020**

Chair: Takehito Nakano

- 09:30 - 9:55            **20-O01**  
High-throughput survey of multicomponent material systems using composition graded materials  
Teruyuki Ikeda (Ibaraki University, Japan)
- 09:55 - 10:20        **20-O02**  
Search for unconventional correlated electrons under chiral symmetry in rare-earth intermetallics  
Kazuaki Iwasa (Ibaraki University, Japan)
- 10:20 - 10:45        **20-O03**  
Magnetic resonance investigation of one-dimensional organic conductors  
Toshikazu Nakamura (Institute of Molecular Science, Japan)
- 10:45 - 11:00        Coffee Break
- 11:00 - 11:25        **20-O04**  
Circularly polarized luminescence due to symmetry breaking  
Yoshitane Imai (Kindai University, Japan)
- 11:25 - 12:15        **20-O05 (Plenary Lecture)**  
Optically switchable helicenes in supramolecular self-assembly and asymmetric catalysis  
Chien-Tien Chen (National Tsing Hua University, Taiwan)
- 12:15 - 13:00        Lunch
- 13:00 - 14:40        **Poster Session 2**
- 14:40 - 15:00        Coffee Break
- 15:00 - 15:25        **20-O06**  
CPL emission from the photo-excited parallel-oriented aryl/aryl dimers  
Yasuyuki Araki (Tohoku University, Japan)
- 15:25 - 15:50        **20-O07**  
Small figure-eight molecules of double-twisted tethered cyclic binaphthyls display enhanced circularly polarized luminescence  
Masashi Hasegawa (Kitasato University, Japan)

Chair: Seiji Mori

Chair: Yoshitane Imai

- 15:50 - 16:15            **20-O08**  
Assessment of spectral similarity and thermal stability of antibody drugs using circular dichroism spectroscopy  
Satoko Suzuki (JASCO, Japan)
- 16:15 - 16:35            **20-O09**  
Light emitting device based on aggregation induced enhanced circularly polarized luminescent chiral perylene diimide derivatives  
Aoba Kanesaka (Ibaraki University, Japan)
- 16:35 - 17:00            Coffee Break
- 17:00 - 17:50            **20-O10** (*Plenary Lecture*)  
Chiral metal-dithiolene complexes and helicene based materials  
Narcis Avarvari (CNRS, Université d'Angers, France)
- 18:00 - 18:50            **20-O11** (*Plenary Lecture*)  
Methylated BEDT- and EDT-TTF chiral conductors  
Flavia Pop (CNRS, Université d'Angers, France)
- Chair: Masashi Hasegawa

**21 November (Sat) 2020**

Chair: Kazuki Ohishi

09:30 - 9:55

**21-O01**

Distorted superconducting nodal line on single Fermi surface in organic superconductor  $\lambda$ -(BETS)<sub>2</sub>GaCl<sub>4</sub>

Dita Puspita Sari (Shibaura Institute of Technology, Japan)

09:55 - 10:20

**21-O02**

$\pi$ -electron magnetism in alkali-metal superoxides

Takashi Kambe (Okayama University, Japan)

10:20 - 10:45

**21-O03**

Complementary use of muons, neutrons and synchrotron radiation –Study of magnetism in arrayed alkali-metal nanoclusters–

Takehito Nakano (Ibaraki University, Japan)

10:45 - 11:00

Coffee Break

Chair: Kazuaki Iwasa

11:00 - 11:20

**21-O04**

Collapse of the two-step energy gap structure and successive enhancement of the in-gap state of Kondo insulator Yb<sub>1-x</sub>R<sub>x</sub>B<sub>12</sub> (R = Ca, Lu, Y, Sc, Zr)

Wataru Matsuhra (Ibaraki University, Japan)

11:20 - 11:45

**21-O05**

The spin textures in chiral magnets probed by small-angle neutron scattering and muon spin rotation

Kazuki Ohishi (CROSS, Japan)

11:45 - 12:10

**21-O06**

Microscopic mechanism of thermal insulation in Si-Ge and heavy-element-doped Heusler alloys

Satoshi Tsutsui (SPring-8 / JASRI, Japan)

12:10 - 12:15

Closing Remarks

12:15 - 13:00

Lunch

## Session of Sakura Science Plan

21 November (Sat) 2020

- 13:00 - 13:05            Opening remarks at the Session of Sakura Science Plan  
Hiroyuki Nishikawa (Chair of Organizing Committee, Ibaraki University, Japan)
- 13:05 - 13:30            Introduction of Ibaraki University, Virtual tour  
Seiji Mori (Ibaraki University, Japan)
- Chair: Panida Surawatanawong
- 13:30 - 13:45            **21-S01**  
Theoretical Studies on Pd-catalyzed enantioselective direct allylation of 2-alkylpyridines at the side chain  $\alpha$ -position  
Kyohei Kawashima (Ibaraki University, Japan)
- Chair: Seiji Mori
- 13:45 - 14:10            **21-S02**  
Mechanisms of C-O bond activation by nickel H-heterocyclic carbene  
Panida Surawatanawong (Mahidol University, Thailand)
- 14:10 - 14:35            **21-S03**  
Computational study on COVID-19 drug repositioning  
Thanyada Rungrotmongkol (Chulalongkorn University, Thailand)
- 14:35 - 14:50            Coffee Break
- Chair: Thanyada Rungrotmongkol
- 14:50 - 15:05            **21-S04**  
Formation and mechanism of Cu(II)- and Ni(II)-phenoxy radical complexes by O<sub>2</sub>  
Takashi Suzuki (Ibaraki University, Japan)
- 15:05 - 15:30            **21-S05**  
Development of novel synthetic methodology of fluorescent compounds and their applications  
Anawat Ajavakom (Chulalongkorn University, Thailand)
- 15:30 - 15:50            **21-S06**  
Hydrogen production from formic acid dehydrogenation over Pd-deposited carbon nanocones: mechanistic insight from a DFT study  
Nuttapon Yodsinsin (Ubon Ratchathani University, Thailand)

- 15:50 - 16:40      **21-S07** (*Plenary Lecture*)  
Understanding the grammar of supramolecular assembly: role of computation and data science  
G. Narahari Sastry (CSIR - North East Institute of Science & Technology, India)
- 16:40                Discussions for future exchanges and concluding remarks of Sakura Science session  
Seiji Mori (Organizing Committee, Ibaraki University, Japan)

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**The ISQBS2020 at Ibaraki University Organizing Committee**

Hiroyuki Nishikawa (Chair)

Takehito Nakano, Seiji Mori, Takahide Yamaguchi

## Poster Program

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-Chirality in Material Science: Current Status and Future Prospects-

### 19 November (Thu) 2020 ([Remo Day-1](#))

- 19-P01 Shoya Kobayashi (Ibaraki University) "Development of a method for coating titanium nitride particles"
- 19-P02 Hien T. T. Lai (VNU University of Science) "hTSP0 monomeric structural model in complex with the PK11195 ligand studied by molecular dynamics simulation"
- 19-P03 Yuki Mimura (Kindai University) "Pyrenylalanine and 2-Aminoisobutanoic Acid (Aib)"
- 19-P04 Chiori Ohgane (Ibaraki University) "An active shield steering magnet for precise control of muon beam in the injection volume"
- 19-P05 Mizuki Ito (Ibaraki University) "Fabrication of silica-coated luminescent particles and their properties"
- 19-P06 Khanittha Kerdpol (Chulalongkorn University) "Conformational study of 3-hydroxyflavone in  $\gamma$ -cyclodextrin inclusion complex"
- 19-P07 Shingo Takahashi (Ibaraki University) "Development of a homogeneous magnetic field coil for the evaluation of a  $^3\text{He}$  neutron spin filter"
- 19-P08 Shota Takashima (Ibaraki University) "OES observation of ZnO molecule in Zn-O<sub>2</sub> mixture plasma"
- 19-P09 Ryohei Kameyama (The University of Tokyo) "The simplified model systems for doped PEDOT (poly(3,4-ethylene dioxythiophene)): EDOT oligomer-based single crystals of radical cation salts"
- 19-P10 Kodai Oda (Ibaraki University) "Beam dynamics study for 3-D spiral injection scheme"
- 19-P11 Sae Wakabayashi (Kyoto Prefectural University) "Synthesis and properties of novel CPP derivatives composed of dinaphtho thiophenes"
- 19-P12 Ami Shimoda, Kazuaki Iwasa (Ibaraki University) "Crystal structure and magnetic property of Nd<sub>3</sub>Rh<sub>4</sub>Sn<sub>13</sub>: a possible chiral magnet"
- 19-P13 Mami Shiozawa, Shiori Suzuki (Ibaraki University) "Atomic substitution effect on chiral structure and superconductivity of La<sub>3</sub>(Co<sub>1-x</sub>Fex)<sub>4</sub>Sn<sub>13</sub> and La<sub>3</sub>(Co<sub>1-x</sub>Ru<sub>x</sub>)<sub>4</sub>Sn<sub>13</sub> "
- 19-P14 Daisuke Hashimoto, Kazuki Gunji (Ibaraki University) "Ru-substitution effect on structural transitions and electronic states in chiral materials Ce<sub>3</sub>Rh<sub>4</sub>Sn<sub>13</sub> and La<sub>3</sub>Rh<sub>4</sub>Sn<sub>13</sub>"
- 19-P15 NA



- 19-P16 Pandey Sadikshya (Tohoku University) "Synthesis and spectroscopic characterization of chiral pyrene dimer"
- 19-P17 Hiroyuki Baba (Ibaraki University) "Muon Knight shift study on alkali-metal clusters in sodalite"
- 19-P18 Takumi Itoh (Ibaraki University) "Structure analyses of Rubrerythrin from *Clostridium acetobutylicum*"
- 19-P19 Tomomasa Hosoya (Ibaraki University) "Photophysical properties of chiral perylene diimide derivatives with long alkyl chains"
- 19-P20 Cong Phuong Cao (VNU University of Science) "Investigating molecular mechanism for the stability of ternary systems containing cetrimide, fatty alcohol and water by using computer simulation"
- 19-P21 Phong Hoang Le (VNU University of Science) "Hydrogen adsorption mechanism of MOF-74 metal organic frameworks: An insight from first principles calculations"
- 19-P22 Daiki Tauchi (Ibaraki University) "Chiral Fe(III) complex composed of tridentate Schiff-base type TTF ligands"
- 19-P23 Nobuyuki Hara (Kindai University) "Inter- and Intra-excimer Circularly Polarized Luminescence (CPL) and Monomer Magnetic Circularly Polarized Luminescence (MCPL) Property Derived From Paracyclophane-pyrene Luminophores"
- 19-P24 Utid Suriya (Chulalongkorn University) "Potentials of Flavonoids for the Treatment of *Clostridium difficile* Infection"

## 20 November (Fri) 2020 ([Remo Day-2](#))

- 20-P01 Takefumi Hosoya (Ibaraki University) "Fabrication of metallic copper and metallic aluminum nanoparticles by electrolysis"
- 20-P02 Kazuki Umemura (Ibaraki University) "In-situ neutron diffraction study of effect of austemper temperature on bainite transformation in low-alloyed TRIP steels"
- 20-P03 Ryoma Fujii (Ibaraki University) "Theoretical Investigation of 1,2-Oxidative Trifluoromethylation of Olefins Catalyzed by Vanadyl complexes"
- 20-P04 Ryosuke Isaka (Ibaraki University) "Synthesis and photophysical properties of chiral perylene diimide derivative with hydrogen bonds"
- 20-P05 Hiroki Matsui (Ibaraki University) "A new environmentally friendly Al-Fe-Si thermoelectric material and its thermoelectric properties"
- 20-P06 Ryuta Yurishima (Ibaraki University) "Examination of the existing range of CrMnFeCoNi high entropy alloys using multiple diffusion method"
- 20-P07 Souichirou Matsuno (Ibaraki University) "Investigation of CH<sub>4</sub> plasma processing for adhesion improvement of carbon-based films on brass. "
- 20-P08 Susumu Kato (Ibaraki University) "Plasma redox effect on Cu/Cu<sub>2</sub>O-PV efficiency improvement"
- 20-P09 Takeru Sakamoto (Ibaraki University) "Synthesis and Characterization of Silica-Coated Gold Nanoparticles for Medical Image"
- 20-P10 Chia-Hao Lu (National Tsing Hua University) "Enantioselective Radical Type, 1,2-Oxy-trifluoromethylation of Olefins Catalyzed by Chiral Vanadyl Complexes"
- 20-P11 Chien-I Lien (National Tsing Hua University) "Enantioselective Radical Type, 1,2-Aryloxy-trifluoromethylation of Olefins Catalyzed by Chiral Vanadyl Complexes"
- 20-P12 Kenta Sato (Kitasato University) "Circularly Polarized Luminescence of A Stereogenic Curved Paraphenylene Anchoring A Chiral Binaphthyl in Solution and Solid State"
- 20-P13 Yuuki Ishida (Kitasato University) "Synthesis and Chiroptical Properties of Helical Oligophenylene Anchoring with Planar Chiral [2.2]Paracyclophane"
- 20-P14 Masakazu Nagata (Ibaraki University) "Synthesis of Ladder-Type Azaborines via Pd-catalyzed C-H Activation-Cyclization Reactions"
- 20-P15 Wijak Yospanya (Tokyo Institute of Technology) "Supramolecular Asymmetric Photochirogenesis of 2-Anthracenecarboxylate Dimers in Chiral Medias: From Synthetic Antibody to Silica Hybrid Nanofibers"
- 20-P16 Koutarou Nakagawa (Ibaraki University) "Study on effect of dislocation strain field and dislocation type on dislocation-strengthening using X-ray diffraction"

- 20-P17 Hiroaki Mitsuizumi (Ibaraki University) "Combined MD and QM/MM Investigation of Hydride Reduction of  $5\alpha$ -dihydrotestosterone Catalyzed by  $3\alpha$ -Hydroxysteroid dehydrogenase"
- 20-P18 Pitchayathida Mee-udorn (Chulalongkorn University) "Inhibitory effect of pyrazolopyran-based inhibitors on Plasmodium serine hydroxymethyltransferases"
- 20-P19 Mattanun Sangkhawasi (Chulalongkorn University) "Structural and dynamical properties of Polyethylene vanillate and Polyethylene terephthalate using molecular dynamics simulation"
- 20-P20 NA
- 20-P21 Hyouma Takemori (Ibaraki University) "Synthesis of rare earth dodecaborides  $Y_{1-x}Pr_xB_{12}$  and rare earth hexaborides  $Sm_{1-x}Tm_xB_6$  under sub-mega bar pressure environment and physical properties"
- 20-P22 Moe Sugita (Ibaraki University) "Precise Magnetic Field Operation of Superconducting Magnet for Beam Capture Using Whole-body MRI Magnet Technology"
- 20-P23 Nawanwat Chainuwong Pattangoon (Chulalongkorn University) "Can SARS-CoV Neutralising Antibodies Repurpose to SARS-CoV-2 Infection?"
- 20-P24 Akihiro Hayashi (Ibaraki University) "Electron spin resonance study on Rb nanoclusters in zeolite A"