

# Program

## ■ Sunday 12 July 2015

13:00-20:00 Registration opens (3rd floor)

18:00-20:00 Welcome reception (3rd floor Conference Room)

## ■ Monday 13 July 2015

08:10- Registration opens (3rd floor)

08:30-09:00 Opening – ICCOSS 2015

**Session 1** Chair: Keiichiro Ogawa

09:00-09:50 **Plenary Lecture - PL1**

New Experimental Techniques for Exploring the Properties of Organic Solids

**KDM Harris**, Cardiff University, UK

09:50-10:10 **O1** Direct Observation of Chemical Reactions in an Interactive Pore by X-rays

**M Kawano**, Pohang University of Science and Technology, Republic of Korea

10:10-10:30 **O2** Fast Molecular Solid-State Reactions by Proper Experimentation

**G Kaupp**, University of Oldenburg, Germany

-Coffee break & Exhibition (3rd floor Conference Room)-

**Session 2** Chair: Kenneth D. M. Harris

11:00-11:50 **Plenary Lecture - PL2**

Chirality in flatland: molecular recognition, chiral switches and unidirectional motors at surfaces

**KH Ernst**, Swiss Federal Laboratories for Materials Science and Technology, Switzerland

11:50-12:10 **O3** Preferential enrichment: Application to racemic compound crystals

**H Takahashi**, Kyoto University, Japan

12:10-12:30 **O4** Chirality Ripening and Crystal to Crystal Conversion

**R Kuroda**, Tokyo University of Science, Japan

-Lunch & Exhibition (3rd floor Conference Room)-

**Session 3** Chair: Hidehiro Uekusa

13:45-14:35 **Plenary Lecture - PL3**

(Including presentation of *ChemComm Emerging Investigator Lectureship 2014*)

2014 ChemComm Emerging Investigator Lecture: Rehabilitating the solid state as a reaction medium - towards a new, green system of chemical synthesis using mechanochemistry

**T Friščić**, McGill University, Canada

- 14:35-14:55 **O5** Sulphur in Crystal Engineering  
**R Bishop**, The University of New South Wales, Australia
- 14:55-15:15 **O6** Cation- $\pi$  Interactions between Pyridinium and Benzene Rings: A Powerful Tool for Arrangement of Organic Molecules  
**S Yamada**, Ochanomizu University, Japan

-Coffee break & Exhibition (3rd floor Conference Room)-

**Session 4**

Chair: Masaki Kawano

- 15:45-16:00 **O7** Engineering ternary cocrystals by orthogonal hydrogen and halogen bonds  
**(Young Scientist Award Presentation)**  
**F Topić**, University of Jyväskylä, Finland
- 16:00-16:15 **O8** Crystal Engineering of Metalloporphyrin Assemblies by Concerted Halogen and Hydrogen Bonding Interactions **(Young Scientist Award Presentation)**  
**HM Titi**, Tel Aviv University, Israel
- 16:15-16:30 **O9** Hydrogen-Bonded Multiporous Hexagonal Networks Composed of  $C_3$ -Symmetric  $\pi$ -Conjugated Macrocycles  
**I Hisaki**, Osaka University, Japan
- 16:30-16:45 **O10** Linking structure with function to design porous organic materials **(Young Scientist Award Presentation)**  
**SY Chong**, University of Liverpool, UK
- 16:45-18:30 **Poster Session 1** <odd numbers> (3rd floor Conference Room)

■ **Tuesday 14 July 2015**

**Session 5**

Chair: Miguel A. Garcia-Garibay

- 09:00-09:50 **Plenary Lecture - PL4**  
Acid-Base Complex Formation to Observe Reaction Intermediates in the Crystalline State  
**Y Ohashi**, Tokyo Institute of Technology, Japan
- 09:50-10:10 **O11** Design of High-performance Supramolecular Host and Guest-dependent Fluorescence Properties of Inclusion Crystals  
**N Tohnai**, Osaka University, Japan
- 10:10-10:30 **O12** Pyridinium-derived zwitterions as supramolecular building blocks  
**DA Haynes**, University of Stellenbosch, South Africa

-Coffee break & Exhibition (3rd floor Conference Room)-

**Session 6**

Chair: Graeme M. Day

- 11:00-11:50 **Plenary Lecture - PL5**  
Amphidynamic Materials and Molecular Machines: Towards Correlated Rotation and Gearing

**MA Garcia-Garibay**, University of California, USA

11:50-12:05 **O13** Crystal Crosslinking as the Third Kind of Crystalline Polymerization  
**K Kokado**, Hokkaido University, Japan

12:05-12:25 **O14** New crystalline phases of Active Pharmaceutical Ingredients obtained by crystallization and heat treatment  
**GD de Delgado**, Universidad de Los Andes, Venezuela

-Lunch & Exhibition (3rd floor Conference Room)-

### **Session 7**

Chair: Akikazu Matsumoto

13:45-14:35 **Plenary Lecture - PL6**  
Photochromism of Diarylethenes in Single Crystals  
**M Irie**, Rikkyo University, Japan

14:35-14:50 **O15** Photomechanical Motion of Benzophenone Crystals  
**H Koshima**, Waseda University, Japan

14:50-15:05 **O16** Photoreversible Current ON/OFF Switching by Photoinduced Bending of Gold-Coated Diarylethene Crystals (**Young Scientist Award Presentation**)  
**D Kitagawa**, Osaka City University, Japan

-Coffee break & Exhibition (3rd floor Conference Room)-

### **Session 8**

Chair: Norimitsu Tohnai

15:35-15:55 **O17** Feedback Mechanisms in Single-Crystal-to-Single-Crystal Solid-State Reactions  
**MA Fernandes**, University of the Witwatersrand, South Africa

15:55-16:10 **O18** Structure-Reactivity Correlations and Mechanistic Understanding of Photoinduced Rearrangement and Photosensitive Effect of  $\alpha$ -Santonin and its Derivatives in Solutions, Crystals and Crystalline Suspensions (**Young Scientist Award Presentation**)  
**P Commins**, University of California–Los Angeles, USA

16:10-16:25 **O19** In situ Control of Solid-State [2+2] Photodimerization in the Dual Photoreactive Crystal  
**A Sekine**, Tokyo Institute of Technology, Japan

16:25-16:40 **O20** Structure and Photoreaction of Unsaturated Carboxylic Acids in the Liquid Crystalline State  
**A Matsumoto**, Osaka Prefecture University, Japan

16:45-18:30 **Poster Session 2** <even numbers> (3rd floor Conference Room)

## **■ Wednesday 15 July 2015**

### **Session 9**

Chair: Graciela Diaz de Delgado

09:00-09:50 **Plenary Lecture - PL7**

Functional Liquid-Crystalline Assemblies Exhibiting Photonic, Ionic, and Separation Properties

**T Kato**, The University of Tokyo, Japan

09:50-10:10 **O21** Ferroelectricity from Molecular Rotation in Organic Ionic Crystals

**J Harada**, Hokkaido University, Japan

10:10-10:30 **O22** Aggregation-induced emission (AIE) behavior of difuroanthra-quinones and their TCNQ analogues

**N Hayashi**, University of Toyama, Japan

-Coffee break & Exhibition (3rd floor Conference Room)-

**Session 10** Chair: Roger Bishop

11:00-11:50 **Plenary Lecture - PL8**

Organic Radical Crystals: From Structural Transformations to Electronic Functions

**K Awaga**, Nagoya University, Japan

11:50-12:10 **O23** Photoinduced Dynamics in Organic Crystals Studied by Time-resolved Vibrational Spectroscopy

**K Onda**, Tokyo Institute of Technology, Japan

-Short break-

12:25-12:40 **O24** Photo-induced dynamics of Me<sub>4</sub>P[Pt(dmit)<sub>2</sub>]<sub>2</sub> studied by time-resolved optical spectroscopy and electron-diffraction technique

**T Ishikawa**, Tokyo Institute of Technology, Japan

12:40-12:55 **O25** High field temperature dependent magneto-photocurrent in organic photo-voltaic cells

**B Khachatryan**, Technion-Israel Institute of Technology, Israel

12:55-13:10 **O26** Re-examination of Amio Acid NCA Polymerization 64. Topochemical Polymerization of L-Glutamic Acid Ester N-Carboxy Anhydrides

**H Kanazawa**, Fukushima University, Japan

-Lunch & Exhibition (3rd floor Conference Room)-

14:00-17:30 Excursion

18:00-20:00 Sushi dinner

## ■ Thursday 16 July 2015

**Session 11** Chair: Kunio Awaga

09:00-09:50 **Plenary Lecture - PL9**

Organic crystal energetics: polymorphism to prediction

**GM Day**, University of Southampton, UK

09:50-10:10 **O27** Analysis of chalcogen-chalcogen and halogen-halogen interactions in crystals

by ab initio molecular orbital calculations

**S Tsuzuki**, National Institute of Advanced Industrial Science and Technology, Japan

10:10-10:25 **O28** Towards computer-guided design of porous molecular organic crystals  
**A Pulido**, University of Southampton, UK

-Coffee break-

**Session 12** Chair: Hiroshi Yamamoto

10:55-11:45 **Plenary Lecture - PL10**

Mechanistic Considerations in Growth Induced Crystal Twisting

**B Kahr**, New York University, USA

11:45-12:05 **O29** Chiral Discrimination in the Solid State: New Ideas on an Old Story

**G Coquerel**, Université de Rouen, France

12:05-12:20 **O30** Construction of Chiral Polar Crystals Composed of Hydrogen-bonded Layers by Halogen Bonds (**Young Scientist Award Presentation**)

**T Sasaki**, Osaka University, Japan

-Lunch-

**Session 13** Chair: Bart Kahr

13:35-14:25 **Plenary Lecture - PL11**

Surface mobility of organic glasses and its role in fast crystallization and formation of stable glasses by vapor deposition

**L Yu**, University of Wisconsin, USA

14:25-14:40 **O31** Continuous preferential crystallization

**C Rougeot**, University of California, USA

14:40-14:55 **O32** Deracemization via Damped Temperature Fluctuations Combined with a Solution Phase Racemization of an Organic Conglomerate Compound

**K Suwannasang**, Suranaree University of Technology, Thailand

-Coffee break-

**Session 14** Chair: Naoto Hayashi

15:25-15:45 **O33** Computational Design of Porous Organic Molecules

**KE Jelfs**, Imperial College London, UK

14:45-16:05 **O34** Colour properties of fluorescein: an interplay of tautomerism and crystal packing (**Young Scientist Award Presentation**)

**M Arhangel'skis**, University of Cambridge, UK

16:05-16:20 **O35** The construction of co-crystal ternary phase diagrams as a tool for solvent selection and design of co-crystallization process with regard to particle size distribution

**J Holoň**, University of Chemistry and Technology Prague, Czech Republic

16:20-16:35 **O36** Solvent vapour-assisted cocrystallisation  
**I Sarceviča**, University of Latvia, Latvia

-Short break-

**Session 15** Chair: Jun Harada

16:55-17:25 **ICDD Sponsored Lecture**

Polymorphism in commercially important pharmaceuticals analyzed using the PDF-4 / Organics database

**GD de Delgado**, Universidad de Los Andes, Venezuela

17:25-17:40 **Young Scientist Awards and Poster Awards**

17:40-18:00 **O37** Thin-Film Single Crystals for Organic Superconducting Transistor

**HM Yamamoto**, Institute for Molecular Science, Japan

18:00-18:15 **O38** On the Headaches of Resolving a Low Melting Combination as a Cocrystal or Eutectic

**S Cherukuvada**, Indian Institute of Science, India

19:30-21:30 Banquet (Hotel Nikko Niigata)

## ■ Friday 17 July 2015

**Session 16** Chair: Hidehiro Uekusa

09:00-09:50 **Plenary Lecture - PL12**

Asymmetric Synthesis Involving Dynamic Preferential Crystallization

**M Sakamoto**, Chiba University, Japan

09:50-10:10 **O39** Dynamic Quantum Crystallography: Refinement of lattice dynamical models from periodic ab-initio calculations against elastic X-ray and neutron diffraction data

**AØ Madsen**, University of Copenhagen, Denmark

10:10-10:25 **O40** Determining the Nature and Properties of the Reflective Materials in the Reflection Superposition Compound Eye (**Young Scientist Award Presentation**)

**BA Palmer**, Weizmann Institute of Science, Israel

-Coffee break-

**Session 17** Chair: Masami Sakamoto

10:55-11:15 **O41** Cryoformation of the New Crystalline Drug Nanostructures

**YN Morozov**, Moscow State University, Russia

11:15-11:30 **O42** Magneto-Structural Correlation in Imidazopyridine Nitronyl Nitroxide Derivatives and Polymorphism

**N Yoshioka**, Keio University, Japan

12:30-12:20 **Plenary Lecture - PL13**

Crystalline Sponge Method Updated: X-ray Details and Applications

**M Fujita**, The University of Tokyo, Japan

12:20-12:30

Conclusion Remarks