

AsCA'13



Hong Kong



The 12th Meeting of the Asian  
Crystallographic Association

7-10 December 2013

The Hong Kong University of Science and Technology

# AsCA'13 - Plenary and Keynote Sessions

## Saturday 7 December 19.30-20.25

19.30-20.25 **Opening Plenary Lecture** Lecture Theatre A

19.30 PL-1 Plenary Lecture 1:  
**CRYSTALLOGRAPHY AND LARGE RESEARCH INFRASTRUCTURES**  
Sine LARSEN *University of Copenhagen, Denmark.* (ASCA130250)

## Sunday 8 December 08.40-10.30

08.40 **Keynote Session 1: Official Welcome** Lecture Theatre A

09.00 KN-1 Keynote Lecture 1:  
**CUCURBITURIL: NEW TRICKS WITH AN OLD MOLECULE**  
Kimoon KIM *POSTECH, Pohang, Korea* (ASCA130343)

09.45 KN-2 Keynote Lecture 2:  
**STRUCTURAL BASIS OF MOLECULAR MECHANISMS OF PROTON-DRIVEN ANTI-PORTERS OF CATIONS AND DRUGS**  
Osamu NUREKI, Tomohiro Nishimasu, Yoshiki Tanaka and Ryuichiro Ishitani  
*University of Tokyo, Japan* (ASCA130243)

## Monday 9 December 08.50-10.35

08.50- 10.35 **Plenary and IYCr2014 Session:** Lecture Theatre A

08.50 PL-2 Plenary Lecture 2:  
**ELECTRIDE: MATERIALS, STRUCTURE AND PROPERTIES**  
Hideo HOSONO *Tokyo Institute of Technology, Yokohama, Japan* (ASCA130342)

09.40 **INTERNATIONAL YEAR OF CRYSTALLOGRAPHY 2014**  
(Gautam Desiraju, Michele Zema, *IUCr*)

10.10 **IYCR2014 ACTIVITIES IN THE ASIA REGION**  
(Various speakers)

# AsCA'13 - Plenary and Keynote Sessions

## Tuesday 10 December

- 08.50- 10.30 **Keynote Session 2:** Lecture Theatre J
- 08.50 KN-3 Keynote Lecture 3:  
**STRUCTURE DETERMINATION OF MOLECULAR SOLIDS FROM POWDER X-RAY  
DIFFRACTION DATA: CURRENT OPPORTUNITIES AND "STATE OF THE ART**  
Kenneth D.M. HARRIS *Univ. Cardiff, U.K. (ASCA130343)*
- 09.45 KN-4 Keynote Lecture 4:  
**BRAGGS' LEGACY: HOW MODERN SCIENCE BENEFITS**  
Judith A.K. HOWARD *Durham Univ., U.K. (ASCA130264)*
- 16.20-18.30 **Final Plenary Session:** Lecture Theatre A
- 16.20-17.20 MS-19 (see p27 for full details)
- 17.20 PL-3 Plenary Lecture 3:  
**CRYSTAL ENGINEERING OF POROUS MATERIAL PLATFORMS**  
Mike ZAWOROTKO <sup>1</sup>*University of South Florida, Tampa, FL, U.S.A.*  
<sup>2</sup>*Univ. Limerick, Ireland (ASCA130032)*
- 18.10 Plans for AsCA'15 and Concluding Remarks

## AsCA'13 - Workshop Schedules:

### Saturday 7 December

Olex2 Asian Workshop	09.00- 17.00	Lecture Theatre K
South China Structural Biology Symposium	09.00-17.30	Lecture Theatre J

### Sunday 8 December

CCP4 Workshop	16.15-18.00	Lecture Theatre K
Bruker APEX2 Workshop	16.15-18.00	Lecture Theatre D

### Monday 9 December

Cambridge Structural Database Workshop	16.15-18.00	Lecture Theatre E
Bruker PROTEUM2 Workshop	16.15-18.00	Room 2612

### Lunch-time Meetings 13.00-13.45

<b>Sunday 8 December</b>	Bruker AXS	Lecture Theatre K
<b>Monday 9 December</b>	Rigaku	Lecture Theatre K

## AsCA'13 - Council Meetings

<b>Monday 9 December</b>	16.00-18.00	Lecture Theatre K
<b>Tuesday 10 December</b>	13.00-14.00	Lecture Theatre K

# South China Structural Biology Symposium

Saturday 7 December 09.00-17.30

08.30 Registration

Session 1 Convenor and Chair: Zhihong GUO, *Hong Kong Univ. Science and Tech.*

09.00 Welcome and Introduction

09.15 S-1 Keynote Lecture 1.  
**STRUCTURE-BASED DRUG DISCOVERY – FROM INFLUENZA VIRUS TO APOPTOSIS**  
Peter COLMAN, Peter E Czabotar, Guillaume Lessene  
*Walter & Eliza Hall Inst. of Med. Research (WEHI), Melbourne, Australia (ASCA130355)*

10.00 S-2 **THE ENGINEERING OF RIBOSOME-INACTIVATING PROTEIN FOR INCREASING ITS SPECIFICITY TOWARD HUMAN IMMUNODEFICIENCY VIRUS INFECTED CELLS**  
Pangchui SHAW, *Chinese Univ. Hong Kong (ASCA130356)*

10.30 Coffee Break

Session 2 Chair: Pangchui SHAW, *Chinese Univ. Hong Kong*

10.50 S-3 **STRUCTURAL INSIGHTS INTO HOST-PATHOGEN SURVIVAL GAMES**  
Se Won SUH, *Seoul National Univ., Korea (ASCA130002)*

11.20 S-4 **STRUCTURAL STUDIES ON SORTING NEXINS**  
Jinsong LIU, Guangzhou Institutes of Biomedicine and Health (GIBH), Chinese Academy of Sciences, China. (ASCA130115)

11.50 S-5 **NOVEL PROTEIN POST-TRANSLATIONAL MODIFICATIONS REVEALED BY THE CRYSTAL STRUCTURE OF SIRT5**  
Quan HAO *Univ. Hong Kong (ASCA130357)*

12.20 Lunch (University Ground Floor Restaurant)

# South China Structural Biology Symposium contd.

Saturday 7 December 09.00-17.30

Session 3 Chair: Quan HAO, *Univ. Hong Kong*

14.00 S-6 Keynote Lecture 2.

**RESIDUE-SPECIFIC PROTEIN FORCE FIELDS AND THEIR APPLICATIONS**

YunDong WU *Peking Univ. Shenzhen, China* (ASCA130254)

14.45 S-7 **INVESTIGATING CONFORMATIONAL CHANGES OF BIOLOGICAL MACROMOLECULES USING KINETIC NETWORK MODELS** Xuhui HUANG, *Hong Kong Univ. Sci. and Tech.* (ASCA130358)

15.15 S-8 **STRUCTURAL BASIS FOR DRUG DISCOVERY TARGETING NUCLEAR RECEPTORS**  
Yong LI, *Xiamen University, Xiamen, China.* (ASCA130251)

15.30 Tea Break

Session 4 Chair: Xuhui HUANG, *Hong Kong Univ. Science and Tech.*

15.50 S-9 **DISSECTING THE ACTIVE SITE OF CLASS A BETA LACTAMASE TO UNCOVER ALTERNATIVE REACTION PATHWAYS** Yanxiang ZHAO, *Polytechnic Univ. Hong Kong.* (ASCA130359)

16.20 S-10 **STRUCTURE-FUNCTIONAL STUDY OF HUMAN PROTEINS THAT REGULATE CELL PROLIFERATION AND DIFFERENTIATION**  
Guang ZHU, *Hong Kong Univ. Science and Tech.* (ASCA130360)

16.50 S-11 **STRUCTURAL INSIGHTS INTO HOW UREASE ACCESSORY PROTEINS FACILITATE MATURATION OF UREASE**  
Kam Bo WONG, *Chinese Univ. of Hong Kong* (ASCA130300)

17.20 S-12 **STRUCTURAL BASIS OF CARGO RECOGNITION MECHANISMS FOR UNUSUAL MYOSINS**  
Zhiyi WEI *South China U.S.T., Shenzhen*

17.50 Final Discussion and Adjournment

# AsCA'13 Oral Program - Microsymposia

## Area 1. Structural Biology

<b>MS-1</b>	<b>Membrane Proteins</b>	Sunday 8 December	10.50-12.50
<b>MS-4</b>	<b>Macromolecular Complexes &amp; Assemblies</b>	Sunday 8 December	14.00-16.00
<b>MS-7A</b>	<b>New Tools and Methods in Structural Biology I</b>	Sunday 8 December	16.15-18.00
<b>MS-7B</b>	<b>New Tools and Methods in Structural Biology II</b>	Monday 9 December	10.50-12.50
<b>MS-10</b>	<b>Drug discovery/Disease-related Proteins</b>	Monday 9 December	14.00-16.00
<b>MS-13</b>	<b>Hot Structures in Biology</b>	Tuesday 10 December	10.50-12.50
<b>MS-16</b>	<b>Enzymes and Enzyme Inhibitors</b>	Tuesday 10 December	14.00-16.00

## Area 2. Chemical Crystallography

<b>MS-2</b>	<b>Metal-Organic Structural Chemistry</b>	Sunday 8 December	10.50-12.50
<b>MS-5</b>	<b>Chemical Crystallography - Structure and Properties</b>	Sunday 8 December	14.00-16.00
<b>MS-8</b>	<b>Dynamic Aspects of Crystals</b>	Monday 9 December	10.50-12.50
<b>MS-11</b>	<b>Magnetic and Conductive Materials</b>	Monday 9 December	14.00-16.00
<b>MS-14</b>	<b>Nano- and Energy Related Materials</b>	Tuesday 10 December	10.50-12.50
<b>MS-17</b>	<b>Crystal Growth and Engineering</b>	Tuesday 10 December	14.00-16.00

## Area 3. Physical Techniques

<b>MS-3</b>	<b>Computation in Crystallography</b>	Sunday 8 December	10.50-12.50
<b>MS-6</b>	<b>Neutron Diffraction</b>	Sunday 8 December	14.00-16.00
<b>MS-9</b>	<b>Charge Density and Electron Diffraction</b>	Monday 9 December	10.50-12.50
<b>MS-12</b>	<b>X-ray Sources and Detectors</b>	Monday 9 December	14.00-16.00
<b>MS-15</b>	<b>X-ray Free Electron Laser (XFEL)</b>	Tuesday 10 December	10.50-12.50
<b>MS-18</b>	<b>Diffraction and Complementary Methods</b>	Tuesday 10 December	14.00-16.00
<b>MS-19</b>	<b>General Interest I (Biol)</b>	Tuesday 10 December	16.20-17.10
<b>MS-20</b>	<b>General Interest II (Chem)</b>	Tuesday 10 December	16.20-17.10

# AsCA'13 - List of Oral Presentations

Sunday 8 December 10.50-12.50

## MS-1 Membrane Proteins Lecture Theatre J

Chair: Peng ZHANG Shanghai Inst. Biol. Sci., China Co-Chair: Alice VRIELINK, UWA, Australia

- 10.50 O1-1 **MODIFICATIONS TO THE PROTEIN DATA BANK (PDB)**  
Genji KURISU, Atsushi NAKAGAWA, Haruki NAKAMURA *Osaka Univ., Japan (ASCA130144)*
- 11.15 O1-2 **KINK CHARACTERIZATION AND KNOWLEDGE-BASED MODELING OF TRANS-MEMBRANE PROTEINS**  
William Bret CHURCH and Tim Werner *University of Sydney, Australia (ASCA130242)*
- 11.40 O1-3 **CRYSTAL STRUCTURE OF AN ENDOTOXIN MODIFYING ENZYME FROM NEISSERIA**  
Alice VRIELINK, Anandhi Anandan and Charlene M. Kahler *Univ. Western Australia, Crawley, Australia (ASCA130058)*
- 12.05 O1-4 **CRYSTAL STRUCTURE OF OXYGEN EVOLVING PHOTOSYSTEM II AT 1.95Å RESOLUTION WITH REDUCED RADIATION DAMAGE**  
Michi SUGA, Fusamichi Akita and Jian-Ren Shen *Okayama University, Japan (ASCA130051)*
- 12.30 O1-5 **STRUCTURAL STUDIES ON THE EXTRACELLULAR DOMAINS OF THE MAMMALIAN PEPTIDE TRANSPORTERS, PEPT1 AND PEPT2.**  
John BEALE, Louise Bird<sup>2</sup>, Ray Owens<sup>2</sup> and Simon Newstead<sup>1</sup> *University of Oxford, U.K.*  
<sup>2</sup>*Rutherford Appleton Laboratory, Harwell, U.K. (ASCA130046)*



Sunday 8 December

10.50-12.50

**MS-2 Metal-Organic Structural Chemistry**

Lecture Theatre E

Chair: Myoung Soo Lah, Ulsan Natl. Inst. Sci. Tech., Korea

Co-Chair: Sue-Lein Wang, Natl. Tsinghua Univ., Taiwan

- 10.50 O2-1 **NEW TEM TECHNIQUES FOR SOLVING UNKNOWN STRUCTURES OF SUBMICRON- AND NANO-SIZED CRYSTALS**  
Xiaodong ZOU *Stockholm Univ., Sweden* (ASCA130234)
- 11.15 O2-2 **CRYSTAL-TO-CRYSTAL TRANSFORMATION OF A ZEOLITIC IMIDAZOLATE FRAMEWORK**  
Jaehon KIM *Soongsil Univ., Seoul, Korea* (ASCA130230)
- 11.40 O2-3 **DESIGN OF NEW METAL-ORGANIC FRAMEWORKS TOWARD MULTIPLE FUNCTIONS**  
Xian-he BU *Nankai Univ., Tianjin, China* (ASCA130200)
- 12.05 O2-4 **EXPLOSIVES SENSING BY NANOSCOPIC ARCHITECTURES AND ORGANIC REACTIONS IN CONFINED NANOSPACE**  
Partha S. MUKHERJEE *IIS Bangalore, India* (ASCA130135)
- 12.30 O2-5 **DESIGN OF COORDINATION NETWORKS USING MULTI-INTERACTIVE LIGAND TP<sup>HAP</sup> VIA WEAK INTERMOLECULAR INTERACTION**  
Tatsuhiro KOJIMA, Tomofumi Yamada,<sup>2</sup> and Masaki Kawano<sup>1</sup> <sup>1</sup>POSTECH, Pohang, Korea and Gifu Univ., Japan (ASCA130023)

Sunday 8 December

10.50-12.50

**MS-3 Computation in Crystallography**

Lecture Theatre K

Chair: Ross PILTZ, ANSTO, Australia Co-Chair: Horst PUSCHMANN, Univ. Durham, U.K.

- 10.50 O3-1 **AMPLE - USING *AB INITIO* PROTEIN STRUCTURE MODELLING TECHNIQUES TO CREATE AND ENHANCE SEARCH MODELS FOR USE IN MOLECULAR REPLACEMENT**  
Ronan KEEGAN<sup>1</sup>, Jaclyn Bibby<sup>2</sup> Jens Thomas<sup>2</sup> Daniel Rigden<sup>2</sup>, Martyn Winn<sup>3</sup> <sup>1</sup>*CCP4, STFC, Harwell*, <sup>2</sup>*University of Liverpool*, <sup>3</sup>*STFC Daresbury Laboratory, Warrington U.K.*  
(ASCA130156)
- 11.15 O3-2 **X-RAY WAVEFUNCTION REFINEMENT – INTRODUCTION, EXAMPLES, VALIDATION**  
Simon GRABOWSKY<sup>1</sup> Magdalena Woinska,<sup>1,2</sup> Joanna M. Bąk,<sup>1,2</sup> Dylan Jayatilaka<sup>1</sup>  
*Univ. Western Australia, Crawley, Australia* <sup>2</sup>*Univ Warsaw, Poland* (ASCA130091)
- 11.40 O3-3 **CHALLENGES AND SOLUTIONS TO ADDING 200 STRUCTURES A DAY INTO THE CAMBRIDGE STRUCTURAL DATABASE**  
Suzanna WARD, Colin R Groom, Matthew Lightfoot and Jenny Field *CCDC, Cambridge, U.K.* (ASCA130161)
- 12.00 O3-4 **A NEW GENERATION OF CCP4 MONOMER LIBRARY BASED ON CRYSTALLOGRAPHY OPEN DATABASE (COD)**  
Fei LONG<sup>1</sup>, Saulius Grazulis<sup>2</sup>, Andrius Merkys<sup>2</sup>, and Garib Murshudov<sup>1</sup> <sup>1</sup>*MRC Lab Cambridge, U.K.* <sup>2</sup>*Vilnius Univ., Lithuania* (ASCA130122)
- 12.20 O3-5 **MODELING MILLISECOND DYNAMICS OF RNA POLYMERASE II TRANSLOCATION AT ATOMIC RESOLUTION USING MARKOV STATE MODELS**  
Fatima PARDO-AVILA, Lintai Da, Daniel Silva and Xuhui Huang *HKUST, Hong Kong*  
(ASCA130077)
- 12.35 O3-6 **MAPPING CRYSTALLINE MOLECULAR GEOMETRIES TO THE CONFORMATIONAL ENERGY LANDSCAPE**  
Hugh P.G. THOMPSON<sup>1</sup> and Graeme M. Day<sup>1,2</sup> <sup>1</sup>*Univ. Cambridge*, and <sup>2</sup>*Univ. Southampton, U.K.* (ASCA130099)

Sunday 8 December

14.00-16.00

**MS-4      Macromolecular Complexes & Assemblies      Lecture Theatre J**

Chair: Ruchi ANAND, IIT, Bombay, India      Co-Chair: Balaji PRAKASH, IIT Kanpur, India

- 14.00    O4-1    **POTENTIAL ANTIBACTERIALS THAT TARGET THE ENZYME BIOTIN PROTEIN LIGASE FROM *STAPHYLOCOCCUS AUREUS***  
Matthew WILCE et al. *Monash Univ., Clayton, Australia* (AsCA130219)
- 14.25    O4-2    **STRUCTURAL BIOLOGY OF MALARIA PARASITE PROTEINS: SOME INSIGHTS**  
Amit SHARMA *ICGEB, New Delhi, India* (AsCA130186)
- 14.50    O4-3    **BINDING OF DAMAGED DNA INDUCES DIMERIZATION OF UV-DAMAGED DNA BINDING PROTEIN (UVDDB): INVESTIGATING THE ROLE OF OLIGOMERIZATION IN CHROMATINIZED DNA REPAIR**  
Joanne I. YEH et al *Univ. Pittsburgh Medical School, PA, U.S.A.* (ASCA130048)
- 15.15    O4-4    **THE CRYSTAL STRUCTURE OF SFPQ REVEALS A POLYVALENT MOLECULAR GLUE FOR HOLDING NUCLEAR BODIES TOGETHER**  
Mihwa Lee, Agata Sadowska, Archa H Fox and Charles S. BOND *Univ. Western Australia, Crawley, Australia* (ASCA130090)
- 15.40    O4-5    **N $\alpha$ -ACETYLATED SIR3 STABILIZES THE CONFORMATION OF A NUCLEOSOME-BINDING LOOP IN THE BAH DOMAIN**  
Qianglin FANG, Dongxue Yang, Mingzhu Wang, Na Yang, Rui-Ming Xu  
*Inst. for Bio-Physics, CAS, Beijing, China* (AsCA130007)

Sunday 8 December

14.00-16.00

**MS-5 Chemical Crystallography - Structure and Properties** Lecture Theatre E

Chair: Edward R.T. Tiekink, Univ. Malaya, Malaysia Co-Chair: Jun Harada, Hokkaido Univ., Japan

- 14.00 O5-1 **CRYSTAL STRUCTURE-FUNCTION RELATIONSHIPS IN POROUS ORGANIC-INORGANIC IONIC CRYSTALS**  
Sayaka UCHIDA *Univ. Tokyo, Japan (ASCA130222)*
- 14.25 O5-2 **KINETIC ASSEMBLY OF POROUS COORDINATION NETWORKS**  
Masaki KAWANO *POSTECH, Pohang, Korea (ASCA130035)*
- 14.50 O5-3 **OLEX2 – ALL YOU NEED FOR SMALL-MOLECULE STRUCTURE DETERMINATION**  
Horst PUSCHMANN and Oleg Dolomanov *Univ. Durham, U.K. (ASCA130107)*
- 15.15 O5-4 **ZN(II), CD(II) AND HG(II) COMPLEXES OF N,N,N-DONOR LIGANDS: METALLOCYCLES VERSUS COORDINATION POLYMERS.**  
Jim SIMPSON<sup>1</sup>, Saeed Dehghanpour<sup>2</sup>, Robabehsadat Tabatabaei<sup>2</sup> <sup>1</sup>*Univ. Otago, Dunedin, New Zealand* and <sup>2</sup>*Alzahra University, Tehran, Iran (ASCA130126)*
- 15.30 O5-5 **CRYSTAL STRUCTURE, LOCAL STRUCTURE AND PHOTOLUMINESCENCE PROPERTY OF KNDW<sub>2</sub>O<sub>8</sub> POLYMORPHS**  
Swetha BHAT<sup>1</sup>, Diptikanta Swain<sup>2</sup>, Chandrabhas Narayana<sup>1,2</sup>, Mikhail Feygenson<sup>3</sup>, Joerg C Neufeind<sup>3</sup> and Nalini G Sundarama<sup>1</sup> <sup>1</sup>*Poornaprajna Inst.* <sup>2</sup>*J. Nehru Centre, Bengaluru, India,* <sup>3</sup>*Oak Ridge National Laboratory, Oak Ridge, TN, U.S.A. (ASCA130190)*
- 15.45 O5-6 **EXPERIMENTAL AND THEORETICAL CHARGE DENSITY ANALYSIS OF BROMOETHYL SULFONIUM TRIFLUOROMETHANE SULFONATE: ATOMIC CHARGES AND THEIR IMPLICATIONS FOR REACTION MECHANISM**  
Magsood AHMED<sup>1,3</sup>, Muhammad Yar<sup>2</sup>, Ayoub Nassour<sup>1</sup>, Benoit Guillot<sup>1</sup>, Christian Jelsch<sup>1</sup> & Claude Lecomte<sup>3</sup> <sup>1</sup>*Islamia University of Bahawalpur,* <sup>2</sup>*COMSATS Inst. Info.Tech., Lahore, Pakistan* and <sup>3</sup>*Université de Lorraine, Nancy, France (ASCA130036)*

Sunday 8 December

14.00-16.00

**MS-6 Neutron Diffraction**

Lecture Theatre K

Chair: Shin-Ae KIM, KAERI, Korea

Co-Chair: Kirrily RULE, ANSTO, Australia

14.00 O6-1 **A NEW NEUTRON SINGLE-CRYSTAL DIFFRACTOMETER WITH CURVED DETECTOR**

Chang-Hee LEE<sup>1</sup>, Yukio Noda<sup>2</sup>, Shin Ae Kim<sup>1</sup>, Myungkook Moon<sup>1</sup>, Yoshihisa Ishikawa<sup>3</sup> and Hiroyuki Kimura<sup>2</sup> <sup>1</sup>KAERI, Daejeon, Korea, <sup>2</sup>Tohoku University, Sendai and <sup>3</sup>KEK, Japan(ASCA130225)

14.25 O6-2 **SIKA: TAIWAN'S COLD NEUTRON TRIPLE-AXIS AT OPAL**

Jason S GARDNER<sup>1,2</sup>, C. M. Wu<sup>1</sup> and G. Deng<sup>3</sup> <sup>1</sup>NSRRC, Hsinchu, <sup>2</sup>National Taiwan Univ., Taipei, Taiwan <sup>3</sup>ANSTO, Lucas Heights, NSW, Australia (ASCA130273)

14.50 O6-3 **KOALA SINGLE-CRYSTAL NEUTRON DIFFRACTOMETER**

Ross O. PILTZ ANSTO, Lucas Heights, NSW, Australia (ASCA130259)

15.15 O6-4 **IT DEPENDS ON HOW YOU SKIN THE CAT. STUDIES OF THE PYROCHLORE-FLUORITE TRANSFORMATION.**

Peter E.R. Blanchard, Brendan J. KENNEDY and Emily Reynolds, Univ. Sydney, NSW Australia (ASCA130131)

15.40 O6-5 **NEUTRON DIFFRACTION STUDIES OF VERY SHORT O-H...O HYDROGEN BONDS INVOLVING AN AMINE OXIDE AND CARBOXYLIC ACIDS**

Yuxin ZHANG<sup>1</sup>, Alison J. Edwards<sup>2</sup>, Fion T-Y. Yeong<sup>1</sup>, Herman H-Y. Sung<sup>1</sup> and Ian D. Williams<sup>1</sup> <sup>1</sup>HKUST, Hong Kong <sup>2</sup>The Bragg Institute, ANSTO, Lucas Heights, Australia (ASCA130258)

Sunday 8 December

16.15-18.00

**MS-7A      New Tools and Methods in Structural Biology I      Lecture Theatre J**

Chair: Quan HAO, Hong Kong University      Co-Chair: Changyong SONG, RIKEN, Japan

16.15    O7-1    **TEMPERATURE-MIMICS-TIME: A DYNAMIC CRYSTALLOGRAPHIC APPROACH TO CAPTURE REACTION INTERMEDIATES**

Xiaojing YANG,<sup>1-3</sup> Xiaoli Zeng<sup>1</sup>, Jane Kuk<sup>2</sup>, Keith Moffat<sup>2</sup>, Kai-Hong Zhao<sup>1</sup> and Zhong Ren  
<sup>1</sup>*Huazhong Agricultural Univ., Wuhan, China.* <sup>2</sup> *Univ. Chicago, U.S.A.* <sup>3</sup> *Renz Research Inc., Westmont IL, U.S.A.* (ASCA130174)

16.40    O7-2    **COMPLEMENTARY APPROACHES IN STRUCTURAL BIOLOGY AND DRUG DISCOVERY**  
Jennifer L. MARTIN *Univ. Queensland, Brisbane, Australia* (ASCA130038)

17.05    O7-3    **HOW TO USE RANDOM MICROSEEDING BEFORE YOU GET YOUR FIRST CRYSTALS**  
Patrick SHAW STEWART *Douglas Instruments, Hungerford, U.K.* (ASCA130310)

17.25    O7-4    **HAPPY MARRIAGES AMONG BIOPHYSICAL TECHNIQUES**  
Kunchithapadam SWAMINATHAN *National Univ. Singapore, Singapore*(ASCA130141)

17.45    O7-5    **ADVANCED CRYSTAL MOUNTING TOOL FOR GAS PRESSURIZATION IMPROVES EFFICIENCY OF XENON-DERIVATIZATION**  
Nobuhiro MIZUNO, Masatomo Makino, Takashi Kumasaka *JASRI-Spring8, Hyogo, Japan* (ASCA130217)

Monday 9 December 10.50-12.50

**MS-7B New Tools and Methods in Structural Biology II** Lecture Theatre J

Chair: Quan HAO, Hong Kong University Co-Chair: Changyong SONG, RIKEN, Japan

10.50 07-6 **FEMTOSECOND CRYSTALLOGRAPHY AT SACLA TARGETING HIGH-RESOLUTION CRYSTAL STRUCTURE DETERMINATION OF LARGE BIOLOGICAL MACROMOLECULES FREE OF RADIATION DAMAGE.**

Hideo AGO et al. *RIKEN SPring-8 Center, Hyogo, Japan* (AsCA130240)

11.15 07-7 **HIGH-RESOLUTION COHERENT DIFFRACTION IMAGING WITH SYNCHROTRON RADIATION AND XFELS**

Huidong JIANG<sup>1</sup>, Jiadong Fan<sup>1</sup>, Jian Zhang<sup>1</sup>, Zhibin Sun<sup>1</sup>, and Changyong Song<sup>2</sup>  
<sup>1</sup>*Shandong University, Jinan, China.* <sup>2</sup>*RIKEN SPring-8 Center, Hyogo, Japan* (AsCA130268)

11.40 07-8 **NANO-SCALE IMAGING OF BIO SPECIMENS WITH COHERENT X-RAY DIFFRACTION MICROSCOPY**

Jaehyun PARK, Marcus Gallagher-Jones<sup>1,2</sup>, Daewoong Nam<sup>1,3</sup>, Sangsoo Kim<sup>1</sup>, Sunam Kim<sup>1</sup> and Changyong Song<sup>1</sup>. <sup>1</sup>*RIKEN SPring-8 Center, Hyogo, Japan* <sup>2</sup>*Univ. Liverpool, U. K.* <sup>3</sup>*POSTECH, Pohang, Korea* (AsCA130191)

12.05 07-9 **SINGLE BIOMOLECULE IMAGING USING FLUORESCENCE POLARIZATION**

Jong-Bong LEE *POSTECH, Pohang, Korea* (AsCA130276)

12.30 07-10 **LOW RESOLUTION MODEL BUILDING AND REFINEMENT TOOLS IN COOT AND REFMAC5**

Andrea Thorn, Rob Nicholls, Paul Emsley, Fei Long and Garib Murshudov  
*MRC Laboratory, Cambridge, UK.* (AsCA130098)

Monday 9 December 10.50-12.50

**MS-8 Dynamic Aspects of Crystals** Lecture Theatre E

Chair: Masaki Kawano, POSTECH, Pohang Korea Co-Chair: Shin-ichi Adachi, KEK, Japan

- 10.50 O8-1 **SOLID STATE STRUCTURAL TRANSFORMATIONS IN COORDINATION POLYMERS**  
J.J. VITTAL<sup>1,2</sup>, Anjana Chanthappalli,<sup>1</sup> Raghav Medishetty,<sup>1</sup> In-Hyeok Park<sup>2</sup> and Shim Sung Lee<sup>2</sup> <sup>1</sup>National University of Singapore, <sup>2</sup>Gyeongsang National University, Jinju, Korea (ASCA130137)
- 11.15 O8-2 **MECHANO-TRIGGERED SINGLE-CRYSTAL-TO-SINGLE-CRYSTAL TRANSFORMATION OF GOLD(I) ISOCYANIDE COMPLEXES**  
Hajime ITO Hokkaido Univ., Japan (ASCA130148)
- 11.40 O8-3 **TIME-RESOLVED STUDIES OF ULTRAFAST DYNAMICS BY MEANS OF PULSED WHITE X-RAY BEAMS**  
Shunsuke NOZAWA, Tokushi Sato, Ayana Tomita, Manabu Hoshino, Shin-ya Koshihara, Shin-ichi Adachi KEK, Tsukuba, Japan (ASCA130229)
- 12.00 O8-4 **AN ADAPTABLE AND DYNAMICALLY POROUS ORGANIC SALT TRAPS UNIQUE TETRAHALIDE DIANIONS**  
Javier MARTI-RUJAS Italian Institute of Technology, Milan, Italy (ASCA130150)
- 12.20 O8-5 **GUEST SORPTION AND RELEASE OF THE MACROCYCLIC BRONIC ESTER POROUS CRYSTALS INVESTIGATED BY AB INITIO STRUCTURE DETERMINATION FROM POWDER DIFFRACTION DATA**  
Hidehiro UEKUSA<sup>1</sup>, Kotaro Fujii<sup>1</sup>, Yuji Kikuchi<sup>2</sup>, Hiroki Takahagi<sup>2</sup>, Kosuke Ono<sup>2</sup>, and Nobuharu Iwasawa<sup>2</sup> Tokyo Inst. Tech., Japan (ASCA130075)
- 12.35 O8-6 **ANOMALOUS THERMAL EXPANSION IN PILLARED-PADDLEWHEEL COORDINATION FRAMEWORKS: MECHANISMS AND APPLICATIONS**  
Yue WU and Cameron J. Kepert Univ. Sydney, Australia (ASCA130139)



Monday 9 December 10.50-12.50

**MS-9 Charge Density and Electron Diffraction** Lecture Theatre K

Chair: P. NAKASHIMA, Monash Univ., Australia Co-Chair: S. GRABOWSKY, Univ. Western Australia

- 10.50 09-1 **STUDY OF NANOSCALE LOCAL STRUCTURES OF FERROELECTRIC BARIUM TITANATE USING CONVERGENT-BEAM ELECTRON DIFFRACTION**  
Kenji TSUDA, Rikiya Sano, Akira Yasuhara and Michiyoshi Tanaka *Tohoku Univ., Japan* (ASCA130065)
- 11.15 09-2 **CHARGE DENSITY DETERMINATION BY CONVERGENT BEAM ELECTRON DIFFRACTION & DFT CALCULATIONS FOR TRANSITION METALS & INTERMETALLICS**  
Jorg WIEZOREK, Xiahn Sang, Andreas Kulovits and Guofeng Wang *Univ. Pittsburgh, PA, U.S.A.* (ASCA130152)
- 11.40 09-3 **HOST-GUEST INTERACTION AND REDUCTION OF THERMAL CONDUCTIVITY IN THERMOELECTRIC MATERIALS OF TYPE-I CLATHRATES**  
Akihiro FUJIWARA<sup>1,2</sup>, Kuniyoshi Sugimoto<sup>1</sup>, Hitoshi Tanaka<sup>3</sup>, Yoichi Tanabe<sup>2</sup>, Satoshi Heguri<sup>2</sup>, Katsumi Tanigaki<sup>2</sup> and Masaki Takata<sup>1,4</sup> <sup>1</sup>Spring-8 Hyogo, <sup>2</sup>Tohoku Univ., Sendai, <sup>3</sup>Shimane Univ., <sup>4</sup>Univ. Tokyo, Japan (ASCA130261)
- 12.00 09-4 **PROBING THE STRUCTURAL, ELECTRICAL AND MECHANICAL BEHAVIORS OF NANOMATERIALS BY ADVANCED TEM TECHNIQUES**  
Jianbo WANG *Wuhan Univ., China* (ASCA130270)
- 12.20 09-5 **THREE DIMENSIONAL INVESTIGATIONS OF DEFORMATION AND RECRYSTALLIZATION STRUCTURES OF METALS BY ELECTRON BACK SCATTER DIFFRACTION TECHNIQUE**  
Zakaria QUADIR, N Afrina, L Bassman<sup>2</sup>, W Xu, P. Munroe and M Ferry *Univ. New South Wales, Sydney, NSW, Australia* <sup>2</sup>Harvey Mudd College, Los Angeles, CA, U.S.A. (ASCA130181)
- 12.35 09-6 **AN INSIGHT INTO THE STRUCTURAL AND BONDING FEATURES OF TETRAARYLCYCLOPENTADIENONES AND RELATED COMPOUNDS THROUGH X-RAY CRYSTALLOGRAPHY AND CHARGE DENSITY ANALYSIS**  
Somnath MUKHERJEE, Sosale Chandrasekhar, Rumpa Paul, T. N. Guru Row *IIS Bangalore, India* (ASCA130017)

Monday 9 December 14.00-16.00

**MS-10 Drug discovery/Disease-related Proteins** Lecture Theatre J

Chair: Peter CZABOTAR, WEHI, Australia Co-Chair: J. SIVARAMAN, NUS, Singapore

- 14.00 O10-1 **SPRING-HAMMER MECHANISM OF METAL ION BINDING AND RELEASE BY THE STREPTOCOCCUS PNEUMONIAE SUBSTRATE-BINDING PROTEIN PSAA**  
Bostjan KOBE et al. *U. Queensland, Brisbane, and Univ. Adelaide, Australia*  
(ASCA130068)
- 14.25 O10-2 **STRUCTURAL BASIS FOR THE NEUTRALIZATION OF HEPATITIS E VIRUS USING MONOCLONAL ANTIBODY**  
Jayaraman SIVARAMAN et al. *National University of Singapore, and Xiamen Univ. China*  
(ASCA130143)
- 14.50 O10-3 **STRUCTURAL BASIS FOR HAEMOGLOBIN CAPTURE BY STAPHYLOCOCCUS AUREUS-STEALING HAEM FROM HAEMOGLOBIN**  
Mitchell GUSS et al. *Univ. Sydney, Univ. Tasmania, WEHI and Australian Synchrotron, Australia, and U.C.L.A., Los Angeles, CA, U.S.A.* (ASCA130050)
- 15.15 O10-4 **CRYSTAL STRUCTURES OF VERTEBRATE DIHYDROPYRIMIDINASE AND COMPLEXES FROM TETRAODON NIGROVIRIDIS WITH LYSINE CARBAMYLATION: METAL AND STRUCTURAL REQUIREMENTS FOR POST-TRANSLATIONAL MODIFICATION AND FUNCTION**  
Chun-Jung CHEN et al *National Synchrotron Radiation Research Center, Hsinchu, Taiwan.*  
(ASCA130187)
- 15.40 O10-5 **STRUCTURE OF SORTING NEXIN 11 (SNX11) REVEALS NOVEL EXTENDED PHOX HOMOLOGY (PX) DOMAIN CRITICAL FOR INHIBITION OF SNX10-INDUCED VACUOLATION**  
Jinxin XU et al. *Guangzhou Inst. of Biomedicine and Health, CAS, Guangzhou, and UST China Hefei* (ASCA130115)

Monday 9 December 14.00-16.00

**MS-11 Magnetic and Conductive Materials** Lecture Theatre E

Chair: R. Murugavel, IIT Bombay, India Co-Chair: Ryoji KIYANAGI J-Parc, JAEA, Japan

- 14.00 O11-1 **CORRELATION BETWEEN STRUCTURE AND OBSERVED MAGNETIC PROPERTIES IN {4F}, {3D-4F} AND {RADICAL-4F} COMPLEXES**  
Saurabh K. Singh, T. Rajeshkumar and Rajaraman GOPALAN *IIT Bombay, Mumbai, India* (ASCA130232)
- 14.25 O11-2 **THE COMPLEX MAGNETIC PHASE DIAGRAM OF THE QUANTUM SPIN CHAIN MATERIAL, LINARITE, PBCUSO<sub>4</sub>(OH)<sub>2</sub>**  
Kirrily Clair RULE<sup>1</sup>, Britta Willenberg,<sup>2,3</sup> Markus Schaeepers,<sup>4</sup> Manfred Reehuis,<sup>2</sup> Anja Wolter-Giraud,<sup>4</sup> Bachir Ouladdiaf,<sup>5</sup> Stefan Suellow<sup>3</sup> <sup>1</sup>*ANSTO, Kirrawee, Australia,* <sup>2</sup>*Helmholtz Centre, Berlin,* <sup>3</sup>*TU Braunschweig,* <sup>4</sup>*Leibniz Institute IFW Dresden, Germany,* <sup>5</sup>*Inst. Laue Langevin, Grenoble, France* (ASCA130087)
- 14.50 O11-3 **HYDROGEN-RELATED PROPERTIES OF METAL AND ALLOY NANOPARTICLES**  
Miho YAMAUCHI *Kyushu Univ. and CREST, Tokyo Japan* (ASCA130145)
- 15.10 O11-4 **STRUCTURE & IONIC CONDUCTION MECHANISM OF LITHIUM SUPERIONIC CONDUCTOR, LI<sub>10</sub>GEP<sub>2</sub>S<sub>12</sub>.**  
Masao YONEMURA<sup>1</sup>, Ohmin Kwon<sup>2</sup>, Masaaki Hirayama<sup>2</sup>, Ryoji Kanno<sup>2</sup>, Yuki Kato<sup>3</sup>, Koji Kawamoto<sup>3</sup>, Shuki Torii<sup>1</sup>, Takashi Kamiyama<sup>1</sup> <sup>1</sup>*KEK, Ibaraki,* <sup>2</sup>*Tokyo Institute of Tech., Yokohama,* <sup>3</sup>*Toyota Motor Corp, Shizuoka, Japan* (ASCA130188)
- 15.30 O11-5 **SPIN CROSSOVER IN A SERIES OF MONONUCLEAR IRON(II) COMPLEXES WITH 4-HALO-N-(2'-PYRIDYLMETHYLENE)ANILINE**  
Kittipong CHAINOK<sup>1</sup>, Songwuit Chanthee<sup>1</sup>, Cindy Mauriac<sup>2</sup>, Philippe Guionneau<sup>2</sup>, and Jean-François Létard<sup>2</sup> <sup>1</sup>*Naresuan Univ., Phitsanulok, Thailand* <sup>2</sup>*Univ. Bordeaux, France* (ASCA130262)
- 15.45 O11-6 **STRUCTURAL AND SODIUM ION MOBILITY STUDIES IN NA<sub>2</sub>MNSIO<sub>4</sub>, A NOVEL CATHODE MATERIAL FOR RECHARGEABLE SODIUM ION BATTERIES**  
Denissa MURPHY and Siegbert Schmid *Univ. Sydney, NSW, Australia* (ASCA130114)

Monday 9 December 14.00-16.00

**MS-12 X-ray Sources and Detectors** Lecture Theatre K

Chair: Sine LARSEN, U. Copenhagen Co-Chair: Herman H-Y. SUNG, Hong Kong

- 14.00 O12-1 **BEAM CONDITIONING IN CUTTING EDGE X-RAY ANALYTICAL EQUIPMENT**  
Jeorg WIESMANN<sup>1</sup>, André Beerlink<sup>1</sup>, Jürgen Graf<sup>1</sup>, Andreas Kleine<sup>1</sup>, Bernd Hasse<sup>1</sup>,  
Carsten Michaelsen<sup>1</sup>, Joachim Lange<sup>2</sup>, and Christoph Ollinger<sup>2</sup> <sup>1</sup>*Incoatec GmbH, Geesthacht*, <sup>2</sup>*Bruker AXS GmbH, Karlsruhe, Germany* (ASCA130026)
- 14.15 O12-2 **ADVANCES IN DATA QUALITY IN AREA DETECTOR DIFFRACTION EXPERIMENTS.**  
Mathias MEYER *Agilent Technologies (Poland) Wrocław, Poland* (ASCA130164)
- 14.30 O12-3 **SHUTTERLESS CMOS DETECTOR DATA PROCESSING USING THE BRUKER APEX2 AND PROTEUM2 SOFTWARE SUITES**  
Eric HOVESTREYDT<sup>1</sup>, Holger Ott<sup>1</sup>, Severine Freisz<sup>1</sup>, Joerg Kaercher<sup>2</sup>, Greg Wachter<sup>2</sup>,  
Stephen Leo<sup>2</sup> <sup>1</sup>*Bruker AXS GmbH, Karlsruhe, Germany* <sup>2</sup>*Bruker AXS Inc., Madison, WI U.S.A.* (ASCA130192)
- 14.45 O12-4 **CURRENT STATUS OF THE LIQUID-METAL-JET X-RAY SOURCE TECHNOLOGY**  
Oscar HEMBERG *Excillum AB, Kista, Sweden* (ASCA130193)
- 15.00 O12-5 **REVISITING S-SAD DATA COLLECTION IN THE HOME LAB: WHAT YOU CAN DO WITH COPPER RADIATION**  
Angela CRISWELL, Mark Del Campo, Pierre Le Magueres, Jim Pflugrath, Joseph D. Ferrara  
*Rigaku Americas Corp., The Woodlands, TX, U.S.A.* (ASCA130207)
- 15.15 O12-6 **GETTING MORE OUT OF YOUR CRYSTALS: DOSE OPTIMIZED MX DATA COLLECTION WITH FAST SINGLE PHOTON COUNTING DETECTORS**  
Clemens SCHULZE-BRIESE *Dectris Ltd., Baden, Switzerland* (ASCA130224)
- 15.30 O12-7 **THE NEW DUAL MODE PIXEL ARRAY DETECTOR**  
Ronald C. HAMLIN<sup>1</sup>, Chris Nielsen<sup>1</sup> and Andrew Arvai<sup>2</sup>  
<sup>1</sup>*Area Detector Systems Corporation, Poway* and <sup>2</sup>*The Scripps Research Institute, La Jolla, CA, U.S.A.* (ASCA130257)

Tuesday 10 December 10.50-12.50

**MS-13 Hot Structures in Biology**

Lecture Theatre J

Chair: Fu GAO, Inst. Microbiol., CAS, Beijing, China

Co-Chair: Shigeyuki YOKOYAMA, Riken, Japan

10.50 O13-1 **TITLE TO BE DETERMINED**

Ruiming XU *IBP, CAS, Beijing, China* (ASCA130354)

11.15 O13-2 **STRUCTURAL BASIS OF THE SPECIFIC RECOGNITION OF THE MAJOR EPITOPE FROM THE JAPANESE CEDAR POLLEN ALLERGEN CRY J 1 BY HLA-DP5**

Seisuke Kusano, Shigeyuki YOKOYAMA et al. *Riken, Saitama, Japan* (ASCA130092)

11.40 O13-3 **FTSZ PROTOFILAMENTS USE A HINGE OPENING MECHANISM FOR CONSTRICTIVE FORCE GENERATION**

Sheng YE *Zhejiang Univ., China* (ASCA130275)

12.00 O13-4 **STRUCTURAL INSIGHTS INTO A NOVEL BACTERIAL C-GMP BINDING DOMAIN REGULATING ITS FUSED DIGUANYLATE CYCLASE GGDEF DOMAIN ACTIVITY**

Shan-Ho CHOU *Natl. Chung Hsing Univ., Taichung, Taiwan* (ASCA130117)

12.20 O13-5 **PLANTS VS. PATHOGENS: STRUCTURAL AND FUNCTIONAL STUDY OF ARABIDOPSIS RESISTANCE PROTEIN SNC1 TIR DOMAIN AND FLAX RUST EFFECTOR PROTEIN AVR-P**

Xiaoxiao ZHANG<sup>1</sup>, Simon Williams<sup>1</sup>, Thomas Ve<sup>1</sup>, Peter N. Dodds<sup>2</sup>, Jeffrey G. Ellis<sup>2</sup> and Bostjan Kobe<sup>1</sup> *<sup>1</sup>Univ. Queensland, Brisbane, <sup>2</sup>CSIRO, Canberra, Australia* (ASCA130083)

12.35 O13-6 **A SELF-GENERATED INTRAMOLECULAR ESTER BOND BETWEEN THR-GLN IN A BACTERIAL CELL SURFACE ADHESIN FROM *CLOSTRIDIUM PERFRINGENS***

Hannah KWON, Christopher J. Squire, Paul G. Young and Edward N. Baker  
*Univ. Auckland, New Zealand* (ASCA130153)

Tuesday 10 December 10.50-12.50

**MS-14 Nano- and Energy Related Materials Lecture Theatre E**

Chair: Miho Yamauchi, Kyushu Univ., Japan Co-Chair: Shin-ichi Adachi, KEK, Japan

10.50 O14-1 **CREATION OF FUNCTIONAL MATERIALS ON THE BASIS OF ELEMENTAL STRATEGY**  
Hiroshi KITAGAWA *Kyoto Univ., Japan (ASCA130155)*

11.15 O14-2 **C<sub>3</sub> SYMMETRIC ORGANIC SYSTEMS FOR MATERIALS CHEMISTRY APPLICATIONS AND PHOSPHATE NANOMATERIALS**  
R. MURUGAVEL, Pratap Bishnoi, Sandeep Kr. Gupta, and Aijaz Ahmed, *IIT Bombay, Mumbai, India (ASCA130142)*

11.40 O14-3 **VISUALIZATION OF THE IONIC CONDUCTION PATHWAY COUPLED BY ELECTROSTATIC INTERACTIONS IN A LAYERED OXIDE**  
Kenichi KATO et al. <sup>1</sup>*RIKEN SPring-8 Center, Hyogo*, <sup>2</sup>*CREST, Japan Science and Technology Agency, Saitama, Japan. (ASCA130340)*

12.05 O14-4 **DEVELOPMENT OF IRON-GROUP NANOALLOY CATALYSTS FOR REALIZATION OF CARBON NEUTRAL SOCIETY**  
Takeshi MATSUMOTO, Masaaki Sadakiyo, Minako Heima, Miho Yamauchi, Tomokazu Yamamoto and Syo Matsumura *Kyushu Univ., Fukuoka, Japan (ASCA130231)*

12.30 O14-5 **NOVEL HYBRID ORGANOPHOSPHATES AS CATHODE MATERIALS FOR LI ION BATTERIES**  
Shahul Hameed ABDULRAHMAN<sup>1</sup>, Mangayarkarasi Nagarathinam<sup>1</sup>, Martin Karl Schreyer<sup>2</sup>, M. V. Reddy<sup>3</sup>, B. V. R. Chowdari<sup>3</sup>, Jagadese J. Vittal<sup>1</sup> *National University of Singapore* <sup>2</sup>*Inst. Chemical & Eng. Sciences, Singapore (ASCA130047)*

Tuesday 10 December 10.50-12.50

**MS-15 X-ray Free Electron Laser (XFEL)**

Lecture Theatre K

Chair: Yoshinori NISHINO, Hokkaido Univ., Japan Co-Chair: Hyunjung KIM, Sogang Univ., Korea

10.50 O15-1 **LONG-RANGE FEMTOSECOND ELECTRONIC CORRELATIONS IN X-RAY LASER NANOCRYSTALLOGRAPHY**

Andrew V. MARTIN<sup>1</sup>, Ruben A. Dilanian<sup>1</sup>, Sophie Williams<sup>1</sup>, Hannah D. Coughlan<sup>2</sup>, Garth J. Williams<sup>3</sup>, Keith A. Nugent<sup>2</sup>, Brian Abbey<sup>2</sup>, and Harry M. Quiney<sup>1</sup> <sup>1</sup>Univ. Melbourne, <sup>2</sup>La Trobe University, Bundoora Australia <sup>3</sup>LiNAC Coherent Light Source, SLAC National Accelerator Laboratory Menlo Park, CA, U.S.A. (ASCA130066)

11.15 O15-2 **DEVELOPMENT OF BIOLOGICAL STRUCTURE-ANALYSIS SYSTEM AT SACLA**

Yasumasa JOTI *SPring8, Hyogo, Japan* (ASCA130088)

11.40 O15-3 **SINGLE-PARTICLE IMAGING WITH X-RAY FREE-ELECTRON LASERS.**

N. Duane LOH<sup>1,2</sup> <sup>1</sup>National University of Singapore, <sup>2</sup>PULSE Institute, SLAC National Laboratory, Menlo Park, CA, U.S.A. (ASCA130123)

12.05 O15-4 **COHERENT DIFFRACTION IMAGING FOR SPHERICAL BIOLOGICAL PARTICLES**

Atsushi NAKAGAWA<sup>1</sup>, Akifumi Higashiura<sup>1</sup>, Kenji Iwasaki<sup>1</sup>, Marina Murakami<sup>1</sup>, Eiki Yamashita<sup>1</sup>, Kazuki Takeda<sup>2</sup>, Yu Hirano<sup>2</sup>, Yuya Hanazono<sup>2</sup>, Kiyofumi Takaba<sup>2</sup>, Masahito Hibi<sup>2</sup>, Yuriko Tomisaki<sup>2</sup>, Kunio Miki<sup>2</sup> <sup>1</sup>Osaka Univ., <sup>2</sup>Kyoto Univ., Japan (ASCA130097)

12.30 O15-5 **CORE-SHELL STRAIN STRUCTURE OF ZSM-5 ZEOLITES BY COHERENT X-RAY DIFFRACTION IMAGING**

Wonsuk CHA et al. *Sogang Univ., Korea* (ASCA130121)

Tuesday 10 December 14.00-16.00

**MS-16 Enzymes and Enzyme Inhibitors** Lecture Theatre J

Chair: Xuhui HUANG, HKUST, Hong Kong Co-Chair: Andrea Thorn, MRC,U.K.

14.00 O16-1 **STRUCTURAL INSIGHTS INTO TRANSCRIPTION MECHANISM OF ANTIBIOTIC REGULATION BY A TETR-FAMILY PROTEIN FROM *STREPTOMYCES COELICOLOR***

Hussain Bhukya and Ruchi ANAND *IIT Bombay, Mumbai, India* (ASCA130149)

14.25 O16-2 **EXPERIMENTAL DEMONSTRATION OF PRODUCT (PYROPHOSPHATE) RELEASE PROVIDED BY STRUCTURAL SNAPSHOTS OF THE URIDYLTRANSFER REACTION CATALYZED BY GLMU**

Balaji PRAKASH, Pravin K.A. Jagtap, Neha Vithani, Sunil Kumar Verma, Vaibhav Bias and Nisanth Nair *Indian Institute of Technology, Kanpur, India*. (ASCA130284)

14.50 O16-3 **CRYSTAL STRUCTURE OF A *BOMBYX MORI* OMEGA-CLASS GLUTATHIONE TRANSFERASE**

Kohji YAMAMOTO<sup>1</sup>, Mamoru Suzuki<sup>2</sup>, Akifumi Higashiura<sup>2</sup> and Atsushi Nakagawa<sup>2</sup>  
<sup>1</sup>*Kyushu Univ., Fukuoka* and <sup>2</sup>*Osaka Univ., Suita Japan* (ASCA130004)

15.15 O16-4 **STRUCTURAL AND FUNCTIONAL STUDIES ON THE REGULATION MECHANISM OF PROTEIN KINASE CK2 BY IP<sub>6</sub> AND NOPP140**

Won-Kyu Lee, Yeon Gyu Yu and Hyung Ho LEE *Kookmin Univ., Seoul, Korea* (ASCA130204)

15.30 O16-5 **IDENTIFICATION OF FUNCTION AND MECHANISTIC INSIGHTS OF GUANINE DEAMINASE**

Aruna BITRA and Ruchi Anand *IIT Bombay, Mumbai, India* (ASCA130031)

15.45 O16-6 **CRYSTAL STRUCTURE OF THE CENTRAL AXIS DF COMPLEX OF *ENTEROCOCCUS HIRAE* V-ATPASE**

K.M. Mozaffor HOSSAIN *Univ. Rajshahi, Bangladesh* (ASCA130024)



Tuesday 10 December 14.00-16.00

**MS-17 Crystal Growth and Engineering** Lecture Theatre E

Chair: Xian-He BU, Nankai Univ., China Co-Chair: Zhengtao XU, City Univ., Hong Kong

- 14.00 O17-1 **ENGINEERING ORGANIC CRYSTALS USING ARENE-PERFLUOROARENE INTERACTIONS**  
Todd B. MARDER *Univ. Würzburg, Germany (ASCA130179)*
- 14.25 O17-2 **SUPRAMOLECULAR AGGREGATION PATTERNS SUSTAINED BY METAL(LONE PAIR)...PI(ARENE) INTERACTIONS**  
Edward R.T. TIEKINK *Univ. Malaya, Malaysia (ASCA130202)*
- 14.45 O17-3 **SULFUR IN THE PORE: TAILORING COORDINATION NETWORKS FOR METAL UPTAKE, SENSING & OTHER APPLICATIONS**  
Zhengtao XU, Jun He, Ka-Kit Yee, Jie Liu *City Univ., Hong Kong (ASCA130310)*
- 15.00 O17-4 **EPITAXIAL AND TOPOTAXIAL GROWTH OF RARE EARTH AND OPTOELECTRONIC NANOMATERIALS**  
Xianfeng Yang, Fenghua Zhao, Jianle Zhuang, Junxiang Fu, Sha Ding, Qiang Zhou,  
Mingmei WU *Sun Yat-Sen Univ., Guangzhou, China (ASCA130348)*
- 15.30 O17-5 **TUNING THE LUMINESCENT SENSING PROPERTIES OF POROUS COORDINATION POLYMERS**  
Xiao-Lin QI, Rui-Biao Lin, Si-Yang Liu, Jie-Peng Zhang and Xiao-Ming Chen *Sun Yat-Sen Univ., Guangzhou, China (ASCA130168)*
- 15.45 O17-6 **ON THE DESIGN AND STRUCTURAL INTER-RELATIONSHIPS OF EUTECTICS AND COCRYSTALS**  
Surya CHERUKUVADA and Tayur N. Guru Row *IIS Bangalore, India (ASCA130178)*

Tuesday 10 December 14.00-16.00

**MS-18 Diffraction and Complementary Methods** Lecture Theatre K

Chair: Alison EDWARDS, ANSTO, Australia

- 14.00 O18-1 **SMALL ANGLE SCATTERING ON THE SUPRAMOLECULAR STRUCTURE DENDRIMER-SURFACTANT COMPLEX IN AQUEOUS SOLUTION**  
Tianfu LI, Yuntao Liu, Dongfeng Chen, Yu Wang, Hongli Wang, Li Zhang, *CIAE, Beijing, China* (ASCA130102)
- 14.25 O18-2 **STRUCTURAL CHARACTERIZATION OF ANISOTROPICALLY STRAINED SNGE THINFILMS USING XRD AND EXAFS**  
Yun-Liang SOO<sup>1,2</sup>, Tai-Sing Wu<sup>1</sup>, Yi-Wei Tsai<sup>1</sup>, Shih-Lin Chang<sup>1,2</sup> and Hung-Hsiang Cheng<sup>3</sup>  
<sup>1</sup>*Natl. Tsing Hua Univ.*, <sup>2</sup>*NSRRC, Hsinchu, Taiwan* <sup>3</sup>*National Taiwan Univ., Taipei, Taiwan* (ASCA130157)
- 14.50 O18-3 **STRUCTURE SOLUTION OF INORGANIC POROUS MATERIALS FROM SINGLE-CRYSTAL XRD, POWDER XRD AND 3D ELECTRON DIFFRACTION**  
Leifeng LIU<sup>1</sup>, Yifeng Yun<sup>1</sup>, Xiaodong Zou<sup>1</sup>, Jihong Yu<sup>3</sup> and Junliang Sun<sup>1,2</sup>  
<sup>1</sup>*Stockholm Univ., Sweden*, <sup>2</sup>*Peking University, Beijing*, <sup>3</sup>*Jilin Univ., Changchun, China* (ASCA130162)
- 15.10 O18-4 **ROLE OF SURFACE AND INTERFACE INTERACTIONS ON THE MOLECULAR STRUCTURE OF BIODEGRADABLE POLY(LACTIDE) STEREOCOMPLEX ULTRATHIN FILMS VIEWED FROM GIXD AND IR-RAS MEASUREMENTS**  
R.R. KUMMETHA, Takahashi Isao, Yukihiro Ozaki *Kwansei Gakuin Univ., Sanda, Japan* (ASCA130170)
- 15.25 O18-5 **METAL COORDINATION POLYMERS OR METAL-ORGANIC FRAMEWORKS FOR ELECTROCHEMICAL APPLICATIONS**  
Chia-Her LIN *Chung Yuan Chr. Univ., Chungli, Taiwan* (ASCA130128)
- 15.45 O18-6 **DYNAMIC ASPECTS ON MOLECULAR CRYSTAL SURFACES**  
Ernest H.H. CHOW, William Jones *Univ. Cambridge, U.K.* (ASCA130163)

Tuesday 10 December 16.20-17.10

**MS-19**      **General Interest Session I (Biol)**      Lecture Theatre A

16.20 O19-1 **ELECTRON DENSITY CONTRIBUTIONS TO THE BATTLE AGAINST SARS AND OTHER ACTUAL DISEASES**  
Peter LUGER *Free University Berlin, Germany (ASCA130283)*

16.45 O19-2 **OVERVIEW OF THE CCP4 SUITE AND CURRENT DEVELOPMENTS**  
Charles BALLARD, Ronan Keegan, Andrey Lebedev, Marcin Wojdyr, Ville Uski, David Waterman and Eugene Krissinel *CCP4, STFC, Harwell, Oxford, U.K. (ASCA130136)*

Tuesday 10 December 16.20-17.10

**MS-20**      **General Interest Session II (Chem)**      Lecture Theatre E

16.20 O20-1 **NEW FORMS OF DRUGS – FROM MECHANOCHEMISTRY TO HIGH PRESSURE**  
Elena BOLDYREVA, *Novosibirsk State University, Russia (ASCA130344)*

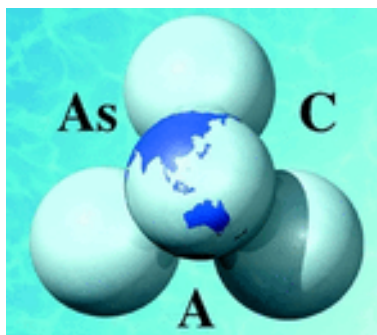
16.45 O20-2 **DRUG DISCOVERY AND DEVELOPMENT BY DESIGN: USING THE KNOWLEDGE FROM EVERY ORGANIC CRYSTAL STRUCTURE EVER PUBLISHED**  
Colin GROOM, Neil Feeder, Elna Pidcock, Peter A. Wood, Peter T.A. Galek and Suzanna Ward *CCDC, Cambridge, U.K. (ASCA130160)*

## Poster Sessions

All abstracts not accepted for Oral presentation are invited for presentation as Posters. Please note the poster board panel size is A0 (90cm wide x 122cm high). It is suggested that posters be printed with some margin for these dimensions (for example 30 x 40 inches). All posters may be displayed from Sunday morning through Monday evening. Presentations will be made during the times indicated. A full list of poster titles, authors and numbers will be posted soon.

<b>Poster Session 1 (odd numbers)</b>	<b>Sunday 8 December</b>	<b>16.15-18.00</b>
<b>Poster Session 2 (even numbers)</b>	<b>Monday 9 December</b>	<b>16.15-18.00</b>

# AsCA'13



# Hong Kong



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