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 ANTIPORTERS 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)
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  \(^1\)*University of South Florida, Tampa, FL, U.S.A.*  
\(^2\)*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
- Sunday 8 December Bruker AXS Lecture Theatre K
- Monday 9 December Rigaku Lecture Theatre K

**AsCA’13 - Council Meetings**
- Monday 9 December 16.00-18.00 Lecture Theatre K
- Tuesday 10 December 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 SIRTS
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
### Area 1. Structural Biology

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<th>MS</th>
<th>Topic</th>
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<tr>
<td>MS-1</td>
<td>Membrane Proteins</td>
<td>Sunday 8 December</td>
<td>10.50-12.50</td>
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<tr>
<td>MS-4</td>
<td>Macromolecular Complexes &amp; Assemblies</td>
<td>Sunday 8 December</td>
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<td>MS-7A</td>
<td>New Tools and Methods in Structural Biology I</td>
<td>Sunday 8 December</td>
<td>16.15-18.00</td>
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<td>MS-7B</td>
<td>New Tools and Methods in Structural Biology II</td>
<td>Monday 9 December</td>
<td>10.50-12.50</td>
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<td>MS-10</td>
<td>Drug discovery/Disease-related Proteins</td>
<td>Monday 9 December</td>
<td>14.00-16.00</td>
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<td>MS-13</td>
<td>Hot Structures in Biology</td>
<td>Tuesday 10 December</td>
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<td>MS-16</td>
<td>Enzymes and Enzyme Inhibitors</td>
<td>Tuesday 10 December</td>
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### Area 2. Chemical Crystallography

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<td>Metal-Organic Structural Chemistry</td>
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<td>MS-5</td>
<td>Chemical Crystallography - Structure and Properties</td>
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<td>14.00-16.00</td>
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<td>MS-8</td>
<td>Dynamic Aspects of Crystals</td>
<td>Monday 9 December</td>
<td>10.50-12.50</td>
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<td>MS-11</td>
<td>Magnetic and Conductive Materials</td>
<td>Monday 9 December</td>
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<td>MS-14</td>
<td>Nano- and Energy Related Materials</td>
<td>Tuesday 10 December</td>
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<td>MS-17</td>
<td>Crystal Growth and Engineering</td>
<td>Tuesday 10 December</td>
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### Area 3. Physical Techniques

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<td>MS-3</td>
<td>Computation in Crystallography</td>
<td>Sunday 8 December</td>
<td>10.50-12.50</td>
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<td>MS-6</td>
<td>Neutron Diffraction</td>
<td>Sunday 8 December</td>
<td>14.00-16.00</td>
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<td>MS-9</td>
<td>Charge Density and Electron Diffraction</td>
<td>Monday 9 December</td>
<td>10.50-12.50</td>
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<td>MS-12</td>
<td>X-ray Sources and Detectors</td>
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<td>MS-15</td>
<td>X-ray Free Electron Laser (XFEL)</td>
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<td>MS-18</td>
<td>Diffraction and Complementary Methods</td>
<td>Tuesday 10 December</td>
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<td>MS-19</td>
<td>General Interest I (Biol)</td>
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<td>16.20-17.10</td>
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<td>MS-20</td>
<td>General Interest II (Chem)</td>
<td>Tuesday 10 December</td>
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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 Bird¹, Ray Owens² and Simon Newstead¹ University of Oxford, U.K. ¹Rutherford 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 TPHAP VIA WEAK INTERMOLECULAR INTERACTION
Tatsuhiro KOJIMA, Tomofumi Yamada, and Masaki Kawano 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  AMPLEx - USING AB INITIO PROTEIN STRUCTURE MODELLING TECHNIQUES TO CREATE AND ENHANCE SEARCH MODELS FOR USE IN MOLECULAR REPLACEMENT
Ronan KEEGAN¹, Jaclyn Bibby², Jens Thomas², Daniel Rigden², Martyn Winn¹ ¹CCP4, STFC, Harwell, ²University of Liverpool, ³STFC Daresbury Laboratory, Warrington U.K. (ASCA130156)

11.15  O3-2  X-RAY WAVEFUNCTION REFINEMENT – INTRODUCTION, EXAMPLES, VALIDATION
Simon GRABOWSKY,¹ Magdalena Woinska,¹,² Joanna M. Bąk,¹,² Dylan Jayatilaka¹
Univ. Western Australia, Crawley, Australia ¹Univ 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 LONG¹, Saulius Grazulis², Andrius Merkys², and Garib Murshudov¹ ¹MRC Lab Cambridge, U.K. ²Vilnius Univ., Lithuania (ASCA130122)

12.20  O3-5  MODELING MILLESECOND 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. THOMPSON¹ and Graeme M. Day¹ ¹Univ. Cambridge, and ²Univ. 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  Nα-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 SIMPSON¹, Saeed Dehghanpour², Robabehsadat Tabatabaei² ¹Univ. Otago, Dunedin, New Zealand and ²Alzahra University, Tehran, Iran (ASCA130126)

15.30  O5-5  **CRYSTAL STRUCTURE, LOCAL STRUCTURE AND PHOTOLUMINESCENCE PROPERTY OF KNDW₂O₈ POLYMORPHS**  
Swetha BHAT¹, Dipktikanta Swain², Chandrabhas Narayana¹,², Mikhail Feygenson³, Joerg C Neuefeind³ and Nalini G Sundarama¹ ¹Poornaprajna Inst. ²J. Nehru Centre, Bengaluru, India, ³Oak 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 AHMED¹,², Muhammad Yar³, Ayoub Nassour¹, Benoit Guillot¹, Christian Jelsch¹ & Claude Lecomte³ ¹Islamia University of Bahawalpur, ²COMSATS Inst. Info.Tech., Lahore, Pakistan and ³Université 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 LEE¹, Yukio Noda², Shin Ae Kim¹, Myungkook Moon¹, Yoshihisa Ishikawa³ and Hiroyuki Kimura² ¹KAERI, Daejeon, Korea, ²Tohoku University, Sendai and ³KEK, Japan (ASCA130225)

14.25 O6-2 **SIKA: TAIWAN’S COLD NEUTRON TRIPLE-AXIS AT OPAL**  
Jason S Gardner¹,², C. M. Wu¹ and G. Deng³ ¹NSRRC, Hsinchu, ²National Taiwan Univ., Taipei, Taiwan ³ANSTO, 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 PYROCHLORO-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 Zhang¹, Alison J. Edwards², Fion T-Y. Yeong¹, Herman H-Y. Sung¹ and Ian D. Williams¹ ¹HKUST, Hong Kong ²The 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,1,3 Xiaoli Zeng1, Jane Kuk2, Keith Moffat2, Kai-Hong Zhao1 and Zhong Ren1  
1Huazhong Agricultural Univ., Wuhan, China. 2 Univ. Chicago, U.S.A. 3 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  O7-6  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  O7-7  HIGH-RESOLUTION COHERENT DIFFRACTION IMAGING WITH SYNCHROTRON RADIATION AND XFELS
Huidong JIANG¹, Jiadong Fan¹, Jian Zhang¹, Zhibin Sun¹, and Changyong Song²
¹Shandong University, Jinan, China. ²RIKEN SPring-8 Center, Hyogo, Japan (AsCA130268)

11.40  O7-8  NANO-SCALE IMAGING OF BIO SPECIMENS WITH COHERENT X-RAY DIFFRACTION MICROSCOPY
Jaehyun PARK, Marcus Gallagher-Jones¹,², Daewoong Nam¹,³, Sangsoo Kim¹, Sunam Kim¹
and Changyong Song¹. ¹RIKEN SPring-8 Center, Hyogo, Japan ²Univ. Liverpool, U. K.
³POSTECH, Pohang, Korea (AsCA130191)

12.05  O7-9  SINGLE BIOMOLECULE IMAGING USING FLUORESCENCE POLARIZATION
Jong-Bong LEE POSTECH, Pohang, Korea (AsCA130276)

12.30  O7-10 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$^{1,2}$, Anjana Chanthappalli$^1$, Raghav Medishetty$^1$, In-Hyeok Park$^2$ and Shim Sung Lee$^{2,3}$
National University of Singapore, $^2$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$^1$, Kotaro Fujii$^1$, Yuji Kikuchi$^2$, Hiroki Takahagi$^2$, Kosuke Ono$^2$, and
Nobuharu Iwasawa$^2$ 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, Xiahan 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 FUJIWARA¹,², Kunihisa Sugimoto¹, Hitoshi Tanaka³, Yoichi Tanabe², Satoshi Heguri³, Katsumi Tanigaki² and Masaki Takata¹,⁴  
¹Spring-8 Hyogo, ²Tohoku Univ., Sendai, ³Shimane Univ., ⁴Univ. Tokyo, Japan (ASCA130261)

12.00 09-4 PROBING THE STRUCTURAL, ELECTRICAL AND MECHANICAL BEHAVIORS OF NANO-MATERIALS 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 Bassman², W Xu, P. Munroe and M Ferry  
Univ. New South Wales, Sydney, NSW, Australia  
²Harvey 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

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, PBCUSO₄(OH)₂**  
Kirrily Clair RULE¹, Britta Willenberg,²,³ Markus Schaepers,² Manfred Reehuis,² Anja Wolter-Giraud,² Bachir Ouladdiaf,⁵ Stefan Suellow³ ¹ANSTO, Kirrawee, Australia, ²Helmholtz Centre, Berlin, ³TU Braunschweig, ⁴Leibniz Institute IFW Dresden, Germany, ⁵Inst. 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, Li₁₀GeP₂S₁₂.**  
Masao YONEMURA¹, Ohmin Kwon², Masaaki Hirayama², Ryoji Kanno², Yuki Kato³, Koji Kawamoto¹, Shuki Torii¹ Takashi Kamiyama¹ ¹²KEK, Ibaraki, ²Tokyo Institute of Tech., Yokohama, ³Toyota Motor Corp, Shizuoka, Japan (ASCA130188)

**15.30 O11-5 SPIN CROSSOVER IN A SERIES OF MONONUCLEAR IRON(II) COMPLEXES WITH 4-HALO-(2'-PYRIDYL METHYLENE)ANILINE**  
Kittipong CHAINOK², Songwuit Chanthee³, Cindy Mauriac², Philippe Guionneau³, and Jean-François Létard² ¹Naresuan Univ., Phitsanulok, Thailand ²Univ. Bordeaux, France (ASCA130262)

**15.45 O11-6 STRUCTURAL AND SODIUM ION MOBILITY STUDIES IN Na₂MNSIO₄, 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, André Beerlink, Jürgen Graf, Andreas Kleine, Bernd Hasse, Carsten Michaelson, Joachim Lange, and Christoph Ollinger. Incoatec GmbH, Geesthacht, Bruker AXS GmbH, Karlsruhe, Germany (ASCA130026)

14.15 O12-2 ADVANCES IN DATA QUALITY IN AREA DETECTOR DIFFRACTION EXPERIMENTS. Mathias MEYER. Agilent Technologies (Poland) Wroclaw, Poland (ASCA130164)

14.30 O12-3 SHUTTERLESS CMOS DETECTOR DATA PROCESSING USING THE BRUKER APEX2 AND PROTEUM2 SOFTWARE SUITES

14.45 O12-4 CURRENT STATUS OF THE LIQUID-METAL-JET X-RAY SOURCE TECHNOLOGY
Oscar HEMBERG. Excilium AB, Kista, Sweden (ASCA130193)

15.00 O12-5 REVISITING S-SAD DATA COLLECTION IN THE HOME LAB: WHAT YOU CAN DO WITH COPPER RADIATION

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, Chris Nielsen and Andrew Arvai. Area Detector Systems Corporation, Poway and 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 CONSTRUCTIVE 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 DIGUANYLA TE 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 ZHANG¹, Simon Williams¹, Thomas Ve¹, Peter N. Dodds², Jeffrey G. Ellis² and Bostjan Kobe¹ ¹Univ. Queensland, Brisbane, ²CSIRO, 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  C₃ 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. ¹RIKEN SPring-8 Center, Hyogo, ²CREST, 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 ON BATTERIES
Shahul Hameed ABDULRAHMAN¹, Mangayarkarasi Nagarathinam¹, Martin Karl Schreyer², M. V. Reddy³, B. V. R. Chowdari³, Jagadese J. Vittal³ National University of Singapore ¹Inst. 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. MARTIN¹, Ruben A. Dilanian¹, Sophie Williams¹, Hannah D. Coughlan²,
Garth J. Williams³, Keith A. Nugent², Brian Abbey³, and Harry M. Quiney¹
¹Univ. Melbourne, ²La Trobe University, Bundoora Australia ³LiNAC 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 SACL
Yasumasa JOTI Spring8, Hyogo, Japan (ASCA130088)

11.40 O15-3 SINGLE-PARTICLE IMAGING WITH X-RAY FREE-ELECTRON LASERS.
N. Duane LOH¹,² ¹National University of Singapore, ²PULSE Institute, SLAC National Laboratory, Menlo Park, CA, U.S.A. (ASCA130123)

12.05 O15-4 COHERENT DIFFRACTION IMAGING FOR SPHERICAL BIOLOGICAL PARTICLES
Atsushi NAKAGAWA¹, Akifumi Higashiura¹, Kenji Iwasaki¹, Marina Murakami¹, Eiki Yamashita¹, Kazuki Takeda², Yu Hirano², Yuya Hanazono², Kiyofumi Takaba², Masahito Hibi², Yuriko Tomisaki², Kunio Miki² ¹Osaka Univ., ²Kyoto 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 URIDYLTTRANSFER 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 YAMAMOTO¹, Mamoru Suzuki², Akifumi Higashiura² and Atsushi Nakagawa²
¹Kyushu Univ., Fukuoka and ²Osaka Univ., Suita Japan (ASCA130004)

15.15  O16-4  STRUCTURAL AND FUNCTIONAL STUDIES ON THE REGULATION MECHANISM OF PROTEIN KINASE CK2 BY IP₆ 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)

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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 Soo1,2, Tai-Sing Wu3, Yi-Wei Tsai1, Shih-Lin Chang1,2 and Hung-Hsiang Cheng3
1Natl. Tsing Hua Univ., 2NSRRC, Hsinchu, Taiwan 3National 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 Liu1, Yifeng Yun1, Xiaodong Zou1, Jihong Yu1 and Junliang Sun1,2
1Stockholm Univ., Sweden, 2Peking University, Beijing, 3Jilin 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
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)

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**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.

Poster Session 1 (odd numbers)  Sunday 8 December  16.15-18.00

Poster Session 2 (even numbers)  Monday 9 December  16.15-18.00
AsCA'13

Hong Kong

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