

**Thursday, October 22**

09:00-12:00 **Meeting Room 1 (2<sup>nd</sup> floor)**

**Workshop 1: Macromolecular crystallization, data collection and data processing techniques**

13:30-17:00 **Meeting Room 1 (2<sup>nd</sup> floor)**

**Workshop 2: Direct-method SAD phasing and dual-space model completion**

13:30-17:00 **Meeting Room 6 (2<sup>nd</sup> floor)**

**Workshop 3: Publication of Small Molecule Structures in IUCr Journals**

18:00-19:00 **Opening and Welcome – IUCr Plenary (Grand Ball Room, 2<sup>nd</sup> floor)**

**Celebrating Crystallography**

Ted Baker

**Chair:** Jianhua Lin

**Friday, October 23**

09:00-09:50 **Grand Ball Room**

Plenary 1

**Vertical Nanowire Arrays: a Universal Platform for Interfacing with Living Cells**

Hongkun Park

**Chair:** Jing-Tai Zhao

09:50-10:10 **Conference Photo**

**October 23, 10:00-12:00 (Grand Ball Room)**

***MS-1 Structural Biology in disease***

**Chairs:** Michael Parker, Xiao-Dong Su

10:00-10:25 **Arms race between host and pathogen**

Jijie Chai

10:25-10:50 **Structural studies of the Glutathione Transferases and their involvement in resistance to chemotherapy treatment.**

Lorien J Parker, Paul J Dyson, Mario Lo Bello, Michael W Parker

10:50-11:15 **Structural Study of PA subunit from an Avian Influenza Virus RNA polymerase**

Yingfang Liu

11:15-11:40 **Ligand recognition by the TLR4-MD-2 complex**

Jie-Oh Lee

11:40-12:00 **Scaffold-based discovery of a novel selective inhibitor of oncogenic B-Raf kinase with potent anti-melanoma activity**  
Kam YJ Zhang

**October 23, 10:00-12:00** (Meeting Room 1, 2<sup>nd</sup> floor)

*MS-2 Inorganic and nano-materials*

**Chairs:** Ian Williams, Stephen S-Y Chui

10:00-10:30 **Metal Organic Frameworks for Proton Conduction and CO<sub>2</sub> Uptake**  
Jeff Hurd, Ramanathan Vaidhyanathan, Jared Taylor, Simon Iremonger, Karl Dawson, George Shimizu

10:30-11:00 **Homoleptic Metal Organothiolate and –selenolate Coordination Polymers [M(SR)<sub>n</sub>]<sub>∞</sub> (n = 1–3): Structural Determination using Powder X-ray Diffraction and Their Materials Properties**  
Stephen Sin-Yin Chui, Kam-Hung Low, Roy VAL, Chi-Ming Che

11:00-11:20 **Ionothermal Synthesis of Metal Organic Framework Materials**  
Zhuojia Lin, Linna Huang, Ming-Liang Tong, Russell E Morris

11:20-11:40 **To bridge or not to bridge – carbonyl ligand configurations in some phosphine and arsine substituted tricobalt carbon cluster systems**  
Jim Simpson, C John McAdam, Brian H Robinson, Roderick G Stanley

11:40-12:00 **Crystal Engineering of Chiral Metal Organic Frameworks (MOFs) from Tartrates and N-Donor Spacer Ligands**  
Pokka K-C Pang, Herman H-Y Sung, Ian D Williams

**October 23, 10:00-12:00** (Meeting Room 6, 2<sup>nd</sup> floor)

*MS-3 Neutron and synchrotron sources and applications*

**Chairs:** Richard Garrett, Hongjie Xu

10:00-10:20 **Current status and future development of neutron scattering at China Advance Research Reactor**  
Dongfeng Chen, Yuntao Liu, Hongli Wang, Kai Sun, Meimei Wu

10:20-10:40 **Current Status of Shanghai Synchrotron Radiation Facility**  
Jianhua He, Zhentang Zhao, Hongjie Xu

10:40-11:00 **Crystallography and Materials Science at the J-PARC pulsed spallation neutron facility**  
Takashi Kamiyama

11:00-11:20 **The Current Status of Taiwan Photon Source**  
Yu Wang, Mau-Tsu Tang, Gwo-Huei Luo, Yaw-Wen Yang, Keng S Liang

11:20-11:40 **Cold Neutron Research Facility at HANARO**  
Kye Hong Lee, Young Ki Kim

11:40-12:00 **New Facilities for Australian Research:  
The Australian Synchrotron and the OPAL Research Reactor**  
Richard F Garrett

**October 23, 12:00-13:30** Rigaku Lunchon Seminar (Grand ball room)

**October 23, 14:00-16:00**

14:00-16:00 **Poster Session 1** (Poster room and corridor on the 2<sup>nd</sup> floor)

**October 23, 16:00-18:30** (Meeting room 1)

*MS-4 Macromolecular assemblies (viruses, proteins, protein-nucleic acid complexes)*

**Chairs:** Peter Metcalf, Tomitake Tsukihara

16:00-16:30 **Structure of the bacterial flagellum and the mechanism of its self-assembly**  
Katsumi Imada

16:30-17:00 **Understanding cytokine receptor signaling**  
Guide Hansen, Tim R Hercus, Jack Kng Scott, Angel F Lopez, Michael W Parker

17:00-17:30 **Effector recognition of Rab and Arf family small G proteins in vesicle transport and membrane remodelling**  
Soichi Wakatsuki

17:30-17:50 **Structural Basis of Transcription: Backtracked RNA Polymerase II**  
Dong Wang, Roger D Kornberg

17:50-18:10 **Structure of RNA-guided RNA Modification Enzymes**  
Keqiong Ye, Ling Li, Jingqi Duan, Ru Jia, Jinzhong Lin, Minghua Ju, Jin Peng, Anbi Xu, Liman Zhang

18:10-18:30 **RNA-protein interactions in the core domain of spliceosomal U4 snRNP**  
Adelaine K W Leung, Jade Li, Kiyoshi Nagai

**October 23, 16:00-18:30** (Meeting Room 6)

*MS-5 Charge density studies*

**Chairs:** Masaki Takata, Yu Wang

16:00-16:30 **Recent Progress in X-ray Charge Density Studies of Advanced Materials**  
Bo B Iversen

16:30-16:55 **Non-linear Optical Properties and Spin Densities from X-ray Charge Density Measurements**  
Dylan Jayatilaka

16:55-17:20 **Exploring Halogen -Halogen interactions via charge density analysis**  
Guru Row

- 17:20-17:45 **Challenge to Atomic Orbital Visualization by 0.2Å Resolution Synchrotron Radiation Single Crystal Experiment**  
Hiroshi Sawa, Eiji Nishibori, Shinobu Aoyagi
- 17:45-18:10 **MEM Electrostatic Potential Imaging**  
Hiroshi Tanaka
- 18:10-18:30 **Photo-induced Structure Determination and Electron Density Study by MEM of Spin Crossover Complex [Fe(abpt)2(NCS)2]**  
Che Hsiu Shih, Chou Fu Sheu, Kunihisa Sugimoto, Jungeun Kim, Kenichi Kato, Yu Wang, Masaki Takata

**October 23, 16:00-18:30 (Meeting Room 7, 2<sup>nd</sup> floor)**

***MS-6 Advanced X-ray/neutron/electron imaging techniques***

**Chairs:** Steve Wilkins, Mau-Tsu Tang

- 16:00-16:30 **Recent Developments in Coherent Diffractive Imaging Instrumentation and Applications**  
Andrew G Peele
- 16:30-17:00 **Visualization of Bio-Structures Using Coherent X-Ray Diffraction**  
Yoshinori Nishino, Kazuhiro Maeshima, Naoko Imamoto, Ryuta Hirohata, Eiichiro Matsubara, Yukio Takahashi, Tetsuya Ishikawa
- 17:00-17:30 **Phase imaging using a liquid cell in a transmission x-ray microscope**  
Gung-Chian Yin
- 17:30-17:50 **Improved Accuracy Laue Neutron Diffraction**  
Ross Piltz, Alison Edwards
- 17:50-18:10 **Development and Application of Neutron 2D-Counter for Crystal and Magnetic Structure Analysis**  
Y Noda, C-H Lee, M-K Moon, S-A Kim, Y Ishikawa, H Kimura, R Kiyonagi
- 18:10-18:30 **State-of-the-art Multilayer Optics for Modern X-ray Analysis**  
J Wiesmann, T Samtleben, C Michaelsen, B Hasse, J Graf, F Hertlein

**Saturday, October 24**

- 09:00-09:50 **Meeting Room 1**  
Keynote 1  
**Proteopedia - a Scientific 'Wiki' Bridging the Rift Between 3D Structure and Function of Biomacromolecules**  
Joel Sussman  
**Chair :** Jenny Martin
- 09:00-09:50 **Meeting Room 6**  
Keynote 2  
**Reactivity and flexibility in metal-organic frameworks: amino-acid based and post-synthetically functionalised materials**

Matthew Rosseinsky  
Chair: Gautam Desiraju

**October 24, 10:00-12:00 (Meeting Room 1)**

***MS-7 Membrane proteins***

Chairs: Jacqui Gulbis, Kenji Inaba

- 10:00-10:25 **Structure and mechanism of an amino acid antiporter**  
Yigong Shi
- 10:25-10:50 **The structure of human connexin 26 gap junction channel**  
Shoji Maeda, So Nakagawa, Michihiro Suga, Eiki Yamashita, Atsunori Oshima, Yoshinori Fujiyoshi, Tomitake Tsukihara
- 10:50-11:15 **The role of AmtB-GlnK complex in nitrogen regulation**  
Xiao-Dan Li, Fritz Winkler, Mike Merrick
- 11:15-11:40 **Structure and function of A-ATPase: combining electron microscopy and X-ray crystallography to study a transmembrane rotary motor complex**  
Lawrence K Lee, Alastair G Stewart, Mhairi Donohoe, Olga Esteban, Ricardo A Bernal, Daniela Stock
- 11:40-12:00 **Crystal Structure of Bacterial Nitric Oxide Reductase, a Key Enzyme in the Respiratory Evolution**  
Yushi Matsumoto, Shingo Nagano, Yoshitsugu Shiro

**October 24, 10:00-12:00 (Meeting Room 6)**

***MS-8 Organic crystal engineering and structure***

Chairs: VR Pedireddi, Suresh Valiyaveetil

- 10:00-10:10 Introduction by Chairs
- 10:10-10:35 **Engineering Organic Crystals using Arene-Perfluoroarene Interactions**  
Todd B Marder
- 10:35-11:00 **Proton Dynamics in Hydrogen-bonded Organic Solids - from Protonic Dielectrics to Proton-motor**  
Tadashi Sugawara, Kentaro Suzuki
- 11:00-11:20 **Structure-property correlations: mechanical properties of molecular crystals**  
C Malla Reddy, Michael T Kirchner, K Anantha Padmanabhan, Gautam R Desiraju
- 11:20-11:40 **Polymorph and pseudo-polymorph of co-crystal; controlling formation and structural transition**  
Miao Du, Xiu-Juan Jiang, Min Tang
- 11:40-12:00 **Towards knowledge-based design and control of pharmaceutical crystal forms**

Colin R Groom, Peter T A Galek, Peter A Wood

**October 24, 10:00-12:00** (Meeting Room 7)

***MS-9 Small angle scattering and soft materials crystallography***

**Chairs:** Naoto Yagi, Monnhor Ree

- 10:00-10:30 **A small/wide-angle X-ray scattering instrument for structural characterizations with soft matter, nanomaterials, and air-liquid interfaces**  
U-Ser Jeng, Chiu Hun Su, Chun-Jen Su, Kuei-Fen Liao, Wei-Tsung Chuang, Ying-Huang Lai, Je-Wei Chang, Yi-Jiun Chen, Yu-Shan Huang, Ming-Tao Lee, Kuan-Li Yu, Din-Goa Liu, Zia-Fung Chang, Chin-Yen Liu, Chien-Hung Chang, Keng S Liang
- 10:30-11:00 **Surface and flow ordering of complex fluids**  
WA Hamilton, L Porcar, PD Butler, GG Warr
- 11:00-11:30 **Intimate Relationship between Micro-phase Separation and Crystalline Phase Transitions in Polyethylene- Poly(ethylene Oxide) Diblock Copolymer as Viewed by Synchrotron SAXS/WAXD and IR/Raman Measurements**  
Kohji Tashiro, Weiyu Cao, Makoto Hanesaka, Hiroyasu Masunaga, Sono Sasaki, Masaki Takata
- 11:30-11:45 **The Quokka Small Angle Neutron Scattering Instrument at OPAL**  
Richard F Garrett, Elliot P Gilbert, William A Hamilton, Kathleen Wood
- 11:45-12:00 **The effect of interface on the crystallization behavior of poly(3-hydroxybutyrate) ultra-thin film revealed by grazing incident X-ray diffraction**  
Xiaoli Sun, Harumi, Sato, Yukihiro Ozaki, Shouke Yan, Isao Takahashi

**October 24, 12:00-13:30** AsCA Council Meeting (Meeting room 3)

**October 24, 14:00-16:00**

14:00-16:00 **Poster Session 2** (Poster room and corridor on the 2<sup>nd</sup> floor)

**October 24 16:00-18:30** (Meeting Room 1)

***MS-10 New tools for macromolecular crystallography (including structural genomics)***

**Chairs:** Kunio Miki, Joel Sussman

- 16:00-16:25 **Tracking ligand migration pathways in carbonmonoxy myoglobin at cryogenic temperatures**  
Shin-ichi Adachi
- 16:25-16:50 **Exploring the conformational energy landscape of acetylcholinesterase by kinetic crystallography**

Jacques-Philippe Colletier, Benoît Sanson, Didier Fournier, Joel L Sussman, Israel Silman, Dominique Bourgeois, Martin Weik

- 16:50-17:10 **Structure of HIV-1 Protease in Complex with Inhibitor KNI-272 Determined by Neutron Crystallography**  
Motoyasu Adachi, Ryota Kuroki
- 17:10-17:30 **Taking the edge off: The softer side of in-house SAD phasing**  
Joseph D. Ferrara, James W. Pflugrath, Cheng Yang
- 17:30-17:50 **Reductive methylation of surface lysines assists crystallization of proteins**  
Neil Shaw, Chongyun Cheng, Zhi-Jie Liu
- 17:50-18:10 **Improvement of a new rotation function for molecular replacement by designing new scoring functions such as relative entropy and dynamic correlation coefficient**  
Fan Jiang, Wei Ding
- 18:10-18:30 **New and Underused Methods for X-ray Crystallography at Low Resolution**  
Yong Xiong

**October 24, 16:00-18:30** (Meeting Room 6)

*MS-11 Metal-organic crystal engineering*

**Chairs:** Ian Williams, Jing-tai Zhao

- 16:00-16:30 **Thermoelectric Zintl Compounds in R-T-Sb (R = Ca, Sr, Ba, Eu, Yb; T = Zn, Cd) Systems**  
XJ Wang, H Zhang, MB Tang, XX Yang, HH Chen, ZY Man, U Burkhardt, Y Grin, JT Zhao
- 16:30-17:00 **Solid-state photochemical reactivity of coordination polymers and metal complexes containing trans-1,2-bis(4-pyridyl)ethylene**  
Jagadese J Vittal, Mangayarkarasi Nagarathinam, Abdul Malik Puthan Peedikakkal
- 17:00-17:25 **Anatomy of a void in an aluminium-copper-tin alloy**  
Laure Bourgeois, Matthew Weyland, Philip NH Nakashima, Barry C Muddle
- 17:25-17:45 **SMART X2S - Chemical Structures at the Touch of a Button**  
Eric Hovestreydt, Michael Ruf, Holger Ott
- 17:45-18:00 **Rational Design, Synthesis and Properties of Layered Compounds LnOZnSb (Ln=La, Ce, Pr, Nd)**  
Kai Guo, Hao-Hong Chen, Zhen-Yong Man, Mei-Bo Tang, Xin-Xin Yang, Xiang-Xin Guo, Jing-Tai Zhao
- 18:00-18:15 **Cation...Cation Supramolecular Interactions in Zinc-Imidazole-Oxovanadate Compounds**  
Samroeng Krachodnok, Kenneth J Haller, Ian D Williams

18:15-18:30 **Synthesis and X-ray Structures of Diorganotin Complexes with *Tris*{(hydroxymethyl)aminomethane Schiff base}**  
See Mun Lee, Hapipah Mohd Ali, Kong Mun Lo

**October 24, 16:00-18:30** (Meeting Room 7)

***MS-12 Powder diffraction***

**Chairs:** Xiaolong Chen, Takashi Ida

16:00-16:25 **Precise Structure Analysis of Ceramic Materials up to 1830 K**  
Masatomo Yashima

16:25-16:50 **Structural analysis of zeolites and related functional materials**  
Yingxia Wang

16:50-17:10 **Spinner-Scan Method for Evaluation of Particle Statistics in Powder Diffractometry**  
Takashi Ida, Taishi Goto, Hisashi Hibino

17:10-17:30 **Structural and magnetic properties of doped wide bandgap semiconductors**  
Gang Wang

17:30-17:50 **Vanadium substituted potassium tungsten bronzes – synthesis and characterization**  
A M Abdullah, A Hussain

17:50-18:10 **Charge density study from high resolution powder diffraction data**  
Eiji Nishibori, Shinobu Aoyagi, Hiroshi Sawa

18:10-18:30 **Interplay between the crystalline and magnetic structures in lightly Cr-doped  $\text{Bi}_{0.37}\text{Ca}_{0.63}\text{Mn}_{0.96}\text{Cr}_{0.04}\text{O}_{2.9}$**   
Wen-Hsien Li, Chun-Chuen Yang, Chun-Ming Wu, Jirong Sun, Jeffrey W Lynn

**Sunday, October 25**

09:00-09:50 **Meeting Room 1**  
Keynote 3  
**Cargo recognition during clathrin-coated vesicle formation**  
David Owen  
**Chair:** Soichi Wakatsuki

09:00-09:50 **Meeting Room 6**  
Keynote 4  
**Crystalline silver(I) complexes containing all-carbon and carbon-rich anionic ligands**  
Thomas Mak  
**Chair:** JJ Vittal

**October 25, 10:00-12:00 (Meeting Room 1)****MS-13 Hot structures****Chairs:** Se-Won Suh, Yigong Shi

- 10:00-10:25 **The structure of rat liver vault**  
Hideaki Tanaka, Koji Kato, Eiki Yamashita, Tomoyuki Sumizawa, Yong Zhou, Min Yao, Kenji Iwasaki, Masato Yoshimura, Tomitake Tsukihara
- 10:25-10:50 **Recognition of Nuclear Export Signal by CRM1**  
Yuh Min Chook
- 10:50-11:15 **NEMO regulates NF- $\kappa$ B activation by specific recognition of linear ubiquitin chains**  
Simin Rahighi, Fumiyo Ikeda, Masato Kawasaki, Masato Akutsu, Nobuhiro Suzuki, Ryuichi Kato, Tobias Kensche, Tamami Uejima, Stuart Bloor, David Komander, Felix Randow, Ivan Dikic, Soichi Wakatsuki
- 11:15-11:40 **The atomic structure of granulovirus polyheir at 1.8Å resolution**  
Elaine Chiu, Shin-Mei Yeh, Richard Bunker, Clemens Schulze-Briese, Peter Metcalf
- 11:40-12:00 **Crystal structure of human REV7 in complex with REV3 fragment**  
Kodai Hara, Toshiyuki Shimizu, Yoshiki Murakumo, Shunsuke Kobayashi, Toshiaki Kogame, Satoko Akashi, Satoru Unzai, Tomo Hanafusa, Haruo Ohmori, Shunichi Takeda, Mamoru Sato, Hiroshi Hashimoto

**October 25, 10:00-12:00 (Meeting Room 6)****MS-14 Superconductivity and crystal properties****Chairs:** Mohana Yethiraj, Xian-Hui Chen

- 10:00-10:40 **High Pressure Synthesis and Superconducting Properties of Oxygen-deficient Oxypnictide Superconductors  $LnFeAsO_{1-y}$**   
H Eisaki, K Miyazawa, M Nakajima, S Ishida, M Ishikado, K Kihou, P M Shirage, C H Lee, N Takeshita, R Kumai, Y Tomioka, H Kito, K M Kojima, T Ito, S Shamoto, S Uchida, A Iyo
- 10:40-11:20 **Diffraction Study of the Fe-based High Temperature Superconductors**  
Wei Bao
- 11:20-11:40 **Electric Polarisation Flop and Magnetic Phase Transition Induced by Magnetic Field in Multiferroic  $RMn_2O_5$  (R=Tm, Yb)**  
Hiroyuki Kimura, Yuma Sakamoto, Mamoru Fukunaga, Yukio Noda, Nobuyuki Abe, Kouji Taniguchi, Taka-hisa Arima, Shuichi Wakimoto, Kazuhisa Kakurai
- 11:40-12:00 **Effect of  $Ga^{3+}$  Substitution for  $Mn^{3+}$  on Magnetic and Dielectric Properties in Multiferroic  $YMn_2O_5$**   
Yuma Sakamoto, Hiroyuki Kimura, Satoru Horio, Arno Fey, Mamoru Fukunaga, Ryoji Kiyonagi, Yukio Noda, Hiraka Haruhiro

**October 25, 16:00-18:30** (Meeting Room 7)***MS-15 Electron microscopy and diffraction*****Chairs:** Laure Bourgeois, Koh Saitoh

- 10:00-10:30 **Electron Microscopy of Low-Dimensional Nanomaterials**  
Fangfang Xu
- 10:30-11:00 **3 Dimensional Coherent Electron Diffractive Imaging of a Nanoparticle**  
Fu-Rong Chen, Roman Dronyak, Keng S Liang
- 11:00-11:30 **High Resolution Structural Analysis of Membrane Proteins by Electron Crystallography**  
Kaoru Mitsuoka
- 11:30-11:45 **Strain Mapping near Si/SiGe Interfaces Using HOLZ Line CBED Patterns**  
Koh Saitoh, Maiko Hamabe, Nobuo Tanaka
- 11:45-12:00 **Visualisation of the Orbital-ordered State of FeCr<sub>2</sub>O<sub>4</sub> using the CBED Method**  
Daisuke Morikawa, Kenji Tsuda, Shintaro Ohtani, Takahisa Arima

**October 25 –12:00-13:30** CCRS Council Meeting (Meeting room 3)**October 25 -13:30-16:35** (Grand Ball Room)

- 13:30-15:30 **Rising Stars Symposium**  
**Chair:** Mitchell Guss
- 15:45-16:35 Plenary 2  
**Structural physiology based on electron crystallography**  
Yoshinori Fujiyoshi  
**Chair:** Zhi-Jie Liu