

Sunday 2nd December

16:00- Registration desk open

20:00

18:00- Halls JK

19:30 Opening Ceremony Welcome Mixer

19:30- PL-1 Hall D

21:00 Special Plenary Lecture

Chair: Prof. Peter Colman, The Walter and Eliza Hall Institute of Medical Research

Multi-crystal Native SAD Analysis of Macromolecular Structure

Prof. Wayne Hendrickson, Columbia University

Monday 3rd December

08:00- Registration desk open

19:30

08:45- PL-2 Hall D

09:45 Plenary 2

Chair: Prof. Keith Nugent, The University of Melbourne

Protein Nano-crystallography with X-ray laser pulses

Prof. Henry Chapman, CFEL DESY

09:45- Halls JK

10:15 Morning tea

10:15- Parallel Sessions 1

12:15

MS-1 - Hall D

Hot structures in Biology

Chairs:

Dr Maria Hrmova, University of Adelaide

Prof. Ian Menz, Flinders University

Invited Speakers: (25+5min presentations)

Structural basis for chaperone-histone interactions

Prof. Ruiming Xu, Chinese Academy of Sciences

Structural Biology of Nuclear Hormone Receptors

Prof. Eric Xu, Van Andel Research Institute

Structure and coupling mechanism of respiratory complex I

Prof. Leo Sazanov, Medical Research Council Mitochondrial Biology Unit

3313 (10+5min Presentation)

The Structural explanations for SNARE selection during clathrin-mediated endocytosis

Dr David Owen, University of Cambridge

3370 (10+5min Presentation)

The Crystal Structure of the Signal Recognition Particle in Complex with its Receptor

Dr Sandro Fernandes Ataide, The University of Sydney

10:15- **MS-2 - MR1**

12:15 **Metallo-organic structural chemistry**

Chairs:

Dr Chris Sumbly, The University of Adelaide

Dr Christian Doonan, The University of Adelaide

Invited Speakers: (25+5min presentations)

Small cyano anions as versatile molecular building blocks

Prof. Stuart Batten, Monash University

Reactivity and Dynamics in Coordination Polymeric Networks

Prof. Jagadeesha J. Vittal, National University of Singapore

3535 (10+5min Presentation)

Crystalline Porous Molecular Solids

Dr. Christian Doonan, The University of Adelaide

3220 (10+5min Presentation)

A Stimuli Responsive System of Anion-Binding Fe₄L₆ Cages

Dr Jack Clegg, The University of Queensland

3102 (10+5min Presentation)

Heterotopic Ligands in Discrete and Polymeric Coordination Compounds

Dr David Turner, Monash University

3034 (10+5min Presentation)

Crystallographic studies of metal[Cu(II), Co(II)] adenine complexes

Mr Yogesh Patil, Indian Institute of Science

10:15- **MS-3 - MR2**

12:15 **Diffraction Physics and applications of crystallography**

Chairs:

Prof Takashi Kamiyama, IMSS/KEK

Dr Andrew Stevenson, CSIRO

Invited Speakers: (25+5min presentations)

X-ray focusing using dynamical diffraction from curved crystal resonator

Prof. Shih-Lin Chang, National Synchrotron Radiation Research Center

Recent challenges of MEM electrostatic potential visualization using SR diffraction data

Prof. Masaki Takata, SPring-8/RIKEN

3153

The current status of versatile neutron diffractometer iMATERIA at J-PARC

Prof Toru Ishigaki, Ibaraki University

3274

Electron vortex pair produced with a nano-fabricated holographic grating

Prof Masaya Uchida, Saitama Institute of Technology

3321

The battle of signal vs noise, and how to tip the balance in your favor
A/Adjunct Prof James Holton, University of California

3340

Determining Changes in Atomic and Electronic Structure of SrTiO₃ Under the
Influence of an External Electric Field

Prof Andrew Johnson, University of Western Australia

12:15- Halls JK

13:30 Lunch

12:15- SCANZ meeting (MR2)

13:30

1300- AsCA Officers Meeting (MR1)

1500

13:30- Halls JK

15:30 Poster Session 1- Even numbers

15:30- Halls JK

16:00 Afternoon tea

16:00- Parallel Sessions 2

18:00

MS-4 - Hall D

Membrane Proteins

Chairs:

Prof. Satoshi Murakami, Tokyo Institute of Technology

Dr. Jacqui Gulbis, The Walter and Eliza Hall Institute of Medical Research

Invited Speakers: (25+5min presentations)

Membrane Protein Structures from a Structural Genomics Approach

Prof. Wayne Hendrickson, Columbia University

Crystallization of membrane proteins using functional antibody fragments

Prof. Takeshi Murata, Chiba University

Electron crystallographic investigations of structures of membrane proteins and
membrane associated proteins

Prof. Alok Mitra, University of Auckland

3130 (10+5min Presentation)

The structure of yeast Ndi1 reveals overlapping binding sites for water- and lipid-
soluble substrates

Dr Megan Maher, La Trobe University

3040 (10+5min Presentation)

The membrane embedded H⁺-translocating pyrophosphatase

Prof. Yuh Ju Sun, National Tsing Hua University

16:00- **MS-5 – MR1**
18:00 **Non-ambient and in-situ Diffraction Studies**

Chairs:

Prof. Hiroshi Fukazawa, JAEA
Prof. Erich Kisi, University of Newcastle

Invited Speakers: (25+5min presentations)

In-situ diffraction techniques for studying hydrogen storage materials under high hydrogen pressure

Prof. Evan Gray, Griffith University

High-pressure neutron diffraction studies of minerals and new beamline at J-PARC
Dr Asami Sano, Japan Atomic Agency

3206 (10+5min Presentation)

High pressure structure and magnetism of one 1-D molecular magnetic material

Dr Jey-Jau Lee, National Synchrotron Radiation Research Center

3212 (10+5min Presentation)

In situ synchrotron studies of carbon dioxide corrosion of mild steel

Bridget Ingham, Industrial Research Ltd

3413 (10+5min Presentation)

Reversible, pressure-induced transformation of the lanthanoid coordination geometry in a highly compressible crystalline solid

Dr Samuel Duyker, Australian Nuclear Science and Technology Organisation

3391 (10+5min Presentation)

Synchrotron and neutron powder diffraction study of incommensurate modulated Ta₂O₅•Al₂O₃

Siegbert Schmid, The University of Sydney

16:00- **MS-6 – MR2**

18:00 **Synchrotron and neutron sources, instrumentation and application**

– *Sponsored by ANSTO*

Chairs:

Prof. Sung-Min Choi, KAIST
Prof. Garry McInyre, Australian Nuclear Science and Technology Organisation

Invited Speakers: (25+5min presentations)

Hard and Fast: developments of diffraction capability at the AS and beyond

Dr Kia Wallwork, Australian Synchrotron Co Lrd

Polarized Neutrons for Advanced Materials Research

Prof. Kazuhisa Kakurai, Japan Atomic Energy Agency

3362 (10+5min Presentation)

Installation and First Beam Tests of the Neutron Image Plate Diffractometer (Bio-C) at HANARO

Shin Ae Kim, Korea Atomic Energy Research Institute

3342 (10+5min Presentation)

Experimental determination of spin dependent electron density by joint refinement of X-ray and polarized neutron diffraction data

Prof. Claude Lecomte, Universite de Lorraine and CNRS

3360 (10+5min Presentation)

Scientific capabilities of the CMCF beamlines at the Canadian Light Source

Dr Pawel Grochulski, Canadian Light Source

3375 (10+5min Presentation)

Development of a New Special Environment Powder Neutron Diffractometer, SPICA

Masao Yonemura, High Energy Accelerator Research Organisation (KEK)

19:20-
21:00 Session 3

MS-6B – Hall D

Diffraction imaging and XFELS

Chairs:

Prof. Hitoshi Tanaka, RIKEN

Prof. Keith Nugent, The University of Melbourne

Invited Speakers: (25+5min presentations)

Opportunities for diffractive imaging at the Linac Coherent Light Source

Dr Garth Jonathan Williams

Coherent Diffractive Imaging at SPring-8 and SACLA

Prof. Yukio Takahashi

Protein crystallography beyond radiation damage limits

Prof. Henry Chapman

3226

Continues X-ray diffractive filed in protein nanocrystallography

Dr Ruben Dilanian, The University of Melbourne

3248

The dynamic Jahn-Teller distortion of C60 induced and observed by interaction with an intense femtosecond X-ray laser pulse

Dr Andrew Martin, The University of Melbourne

Tuesday 4th December

08:00- Registration desk open

18:30

08:45- KN-1

09:45 Hall D

Keynote 1

Chair: Prof. Jenny Martin, University of Queensland

The Natural Killer Cell Receptor 3DL1 – Looking for missing self

Dr Julian Vivian, Monash University

08:45- KN-2

09:45 MR1&2

Keynote 2

Chair: Prof. Ray Withers, Australian National University

Exploring the Hierarchy and Architecture of Solid Solutions with Atom Probe

Microscopy

Prof. Simon Ringer, The University of Sydney

09:45- Halls JK

10:15 Morning Tea

10:15- Parallel Sessions 4

12:15

MS-13 – Hall D

Drug discovery

Chairs:

Dr Kam Zhang, RIKEN

Dr Tom Peat, CSIRO

Invited Speakers: (25+5min presentations)

Structural insights into the mechanism of action of a BACE1 antibody

Dr Weiru Wang, Genentech Inc.

The discovery of Non-ATP site inhibitors of kinases

Dr Sandra Jacob, Novartis Institutes for Biomedical Research

Structure-based design of highly selective phosphodiesterase inhibitors for CNS indications

Dr Jay Pandit, Pfizer Inc

3025 (10+5min Presentation)

BHRF1 inhibition with peptido-mimetics

Dr Sofia Caria, La Trobe University

3035 (10+5min Presentation)

Biologically active 1, 9-Pyrazoloanthrone Derivatives towards Inhibition of c-JNK

Mr Durga Prasad Karothu, Indian Institute of Science

10:15- **MS-8 – MR2**

12:15 **Energy related materials**

Chairs:

Prof. Myung Hyun Paik Suh, Seoul National University

Dr Vanessa Peterson, Australian Nuclear Science and Technology Organisation

Invited Speakers: (25+5min presentations)

Functionalization of metal-organic frameworks for potential applications

Prof. Hongcai (Joe) Zhou, Texas A&M University

Fast ion transport and structural stability of solid lithium ion conductors: insight from combining in situ diffraction with bond-valence based simulations

A/Prof. Stefan Adams, National University of Singapore

2989 (10+5min Presentation)

Structure, thermal and physical properties of spinel type LiMnTiO₄

Ms Denissa Murphy, The University of Sydney

3047 (10+5min Presentation)

Oxide-ionic conduction and the (3+3)-D incommensurately modulated structure of Type II Bi₂O₃-Nb₂O₅

A/Prof. Chris Ling, The University of Sydney

3291 (10+5min Presentation)

Repeated gas adsorption in zeolites for solar cooling applications investigated by Modulation Enhanced Diffraction

Prof. Davide Viterbo, Università del Piemonte Orientale

3418 (10+5min Presentation)

Materials Discovery of Dyes for Dye-Sensitized Solar Cells: Prediction, Validation and Rationalisation

Prof. Jacqueline Cole, University of Cambridge

10:15- **MS-9 – MR2**

12:15 **Dynamic aspects of molecular and solid state crystals**

Chairs:

Prof. Masaki Takata, SPring-8/RIKEN

A/Prof. Chris Ling, The University of Sydney

Invited Speakers: (25+5min presentations)

Simultaneous Measurements of Picosecond Lattice and Charge Dynamics in Co-Fe Cyanides

A/Prof. Yutaka Moritomo, University of Tsukuba

Simulation of disorder and dynamics - from minerals to fuel cells

Prof. Julian Gale, Curtin University

Atomic Dynamics using Sychrotron Radiation: Phonon Softening in Multiferroic EuTiO₃

Dr Alfred Baron, RIKEN SPring-8 Center

3259 (10+5min Presentation)

Pseudo-polymorphic Phase Transition of Pharmaceutical Crystals Revealed by SDPD Method

Dr Hidehiro Uekusa, Tokyo Institute of Technology

3221 (10+5min Presentation)

Diffraction and spectroscopic studies on the pyrochlore-fluorite phase transformation in Ln₂Hf₂O₇ (Ln = lanthanide)

Dr Peter Blanchard, The University of Sydney

12:15- Halls JK

13:30 Lunch

12:30- **Workshop** – Hall D

13:30 Phaser Crystallographic Software run by Dr. Airlie McCoy

13:00- AsCA Council Meeting (MR1)

15:00

13:30- Halls JK

15:30 Poster Session 2- Odd numbers

15:30- Halls JK

16:00 Afternoon Tea

16:00- Parallel Sessions 5

18:00

MS-10 – Hall D

Macromolecular assemblies (Viral proteins)

Chairs:

Prof. Cheng Yang, Tianjin International Academy of Biotechnology and Medicine

Dr Mike Lawrence, The Walter and Eliza Hall Institute of Medical Research

Invited Speakers:

(20+5min presentations)

Structural and functional analysis of the innate immune signaling adaptor protein STING and its potential for drug discovery

Prof. Zhijie Liu, Chinese Academy of Sciences

(20+5min presentations)

The molecular organisation of viral in vivo crystals: arms and armours of insect poxviruses

Dr Fasseli Coulibaly, Monash University

(15+5min presentations)

Crimean–Congo hemorrhagic fever virus nucleoprotein reveals endonuclease activity in bunyaviruses

A/Prof. Zhiyong Lou, Tsinghua University

(15+5min presentations)

Probing Allostery Through DNA - Single molecule and structural studies on several DNA-protein complexes

Prof. Xiao-Dong Su, Peking University

3273 (10+5min Presentation)

Update on the chemokine binding protein from orf virus

Prof. Kurt Krause, University of Otago

3123 (10+5min Presentation)

Role of Domain swapping interactions in the Stationary Phase Survival Protein SurE from *Salmonella typhimurium*

Yamuna Kalyani Mathiharan, Indian Institute of Science

16:00- **MS-11** – MR1

18:00 **Chemical crystallography**

Chairs:

Prof. Yu Wang, National Taiwan University

Prof. Stuart Batten, Monash University

Invited Speakers: (25+5min Presentations)

Crystal Structures of Mesoporous Inorganic Frameworks

Prof. Sue-Lein Wang, National Tsing Hua University

Multi-bistable metal complexes

Prof. Hiroki Oshio, University of Tsukuba

3154 (10+5min Presentation)

In-situ Control of Photochromism of Hybrid Type Cobalt Complexes using Crystalline-State Photoisomerization

Dr Akiko Sekine, Tokyo Institute of Technology

3433 (10+5min Presentation)

Application of the Structure Correlation Principle to Concerted and Stepwise retro Diels Alder Reactions

A/Prof. Jonathan White, University of Melbourne

3372 (10+5min Presentation)

Accurate Chemical Characterization – Fascinating Discoveries and Proofs

Dr Alison Edwards, Australian Nuclear Science and Technology Organisation

3134 (10+5min Presentation)

Crystal Packing Predictions: which are the dominant interactions?

Dr Graeme Gainsford, Industrial Research Limited

16:00- **MS-12** – MR2

18:00 **Structural proteomics and bioinformatics**

Chairs:

Prof. Haruki Nakamura, Osaka University

Prof. Bostjan Kobe, University of Queensland

Invited Speakers: (20+5min Presentation)

Structural genomics of mobile gene elements: Defining protein functions engaged in lateral gene transfer

A/Prof Bridget Mabbut, Macquarie University

Structures of autophagic molecules for autophagosome formation

Prof Hyun Kyu Song, Korea University

Changes in protein-protein interface brought about by complex formation
Prof Pinak Chakrabarti, Bose Institute

Using informatics to straddle the expertise gap in protein crystallogenesi
Dr Janet Newman, CSIRO

3299 (15+5min Presentation)

Error estimation guided rebuilding of de novo models increases the success rate for ab
initio phasing

Dr Kam Zhang, RIKEN

18:00- Awards Ceremony

19:30 Poster Prizes

Wednesday 5th December

08:00- Registration desk open

17:30

08:45- KN-3

09:45 Hall D

Keynote 3

Chair: Prof. John Carver, University of Adelaide

In situ photo-crystallography discovers optoelectronic applications

Prof Jacqueline Cole, University of Cambridge

KN-4 MR1&2

Keynote 4

Chair: Dr Alison Edwards, Australian Nuclear Science and Technology Organisation

Polar nanoregions and diffuse scattering in the relaxor ferroelectrics

Richard Welberry, Australian National University

09:45- Hall JK

10:15 Morning Tea

10:15- Parallel Session 6

12:15

MS-7 – Hall D

Enzymes

Chairs:

Prof. Zihé Rao, Nankai University/Tsing Hua University

Dr Chris Squire, The University of Auckland

Invited Speakers: (25+5min Presentations)

A tale of two cooperative mechanisms of phosphagen kinases: dimeric single-domain and monomeric double-domain

Dr Sheng Ye, Chinese Academy of Sciences

The X-ray Crystal Structure Of Full Length Human Plasminogen

Prof. James Whisstock, Monash University

3022 (15+5min Presentation)

Protein motions and CO migration following CO photolysis in haem oxygenase

A/Prof Masakazu Sugishima, Kurume University School of Medicine

3382 (15+5min Presentation)

Crystal Structure of Auxin Amido Synthetase from Cabernet Sauvignon

Dr Tom Peat, CSIRO

3163 (15+5min Presentation)

Structural analysis of the electron transfer complex between Ferredoxin and

Ferredoxin-dependent glutamate synthase

Dr Kanako Shinmura, Osaka University

10:15- **MS-14 – MR1**

12:15 **Small angle scattering**

Chairs:

Prof Moonhor Ree, Pohang Institute of Science

Dr Charlotte Conn, CSIRO

Invited Speakers: (25+5min Presentations)

Small angle X-ray scattering studies of high-energy ion tracks

Prof. Patrick Kluth, Australian National University

Investigating the Nanoscale Structure in Self-Assembled Polymers, Films and Composites

Prof. Kevin Jack, Centre for Microscopy and Microanalysis

3358 (10+5min Presentation)

High Throughput Biological SAXS for the Home Laboratory

Ms Angela Criswell, Rigaku

3396 (10+5min Presentation)

The solution structure of full length human ezrin by SAXS and protein crystallography

Dr Anthony Duff, Australian Nuclear Science and Technology Organisation

3085 (10+5min Presentation)

The regulatory role of Munc18 proteins in SNARE mediated membrane fusion

Dr Andrew Whitten, University of Queensland

2980 (10+5min Presentation)

The Role of Small-Angle X-Ray and Neutron Scattering Techniques in Understanding Starch Structure

Elliot Gilbert

10:15- **MS-15 – MR2**

12:15 **Crystal growth and engineering**

Chairs:

Prof. Ashwini Nangia, University of Hyderabad

Dr Janet Newman, CSIRO

Invited Speakers: (25+5min Presentations)

Evaluation of Crystal Form using CSD derived Full Interaction Maps

Dr Peter Wood

Engineering proteins and complexes for enhanced crystallizability

Prof. Zygmunt S. Derewenda, University of Virginia

3365 (15+5min Presentation)

An Approach to Crystallizing Proteins by Metal-mediated Synthetic Symmetrization

Ms Angela Soriaga, UCLA

3427 (15+5min Presentation)

Solvothermal Synthesis of Mixed Imidazolate-Benzimidazolate MOFs

Prof. Ian Williams, HKUST

3122 (15+5min Presentation)

X-ray transparent plates for high throughput protein crystallization and diffraction screening

Prof Robert Thorne, Cornell University

12:15- Halls JK

13:30 Lunch

12:15- SCANZ Members AGM (MR2)

14:15

13:00- AsCA Council Meeting 2 (MR1)

15:00

14:10- Hall D

15:30 AsCA/SCANZ Rising Stars Symposium MS

15:30- Halls JK

16:00 Afternoon Tea

15:45- Responding to new era of crystallographic-based science and changes in its global distribution

16:00

Prof. Samar Hasnain, University of Liverpool

16:00- **Hall D**

17:00 **PL-3**

Plenary 3

Chair: Dr Chris Sumby, University of Adelaide

Invited Speaker:

Metal Azolate Frameworks: from Crystal Engineering to Functional Materials

Prof. Xiao-Ming Chen, Sun Yat-Sen University

17:00- Hall D

17:30 Closing Ceremony

18:30- Conference Dinner, National Wine Centre of Australia

23:00