

AsCA 2018 / CRYSTAL 32 SPEAKER TIMETABLE:

SUNDAY DECEMBER 2:

08:00 – 09:00 Registration

08:30 – 09:00 Morning Tea – WORKSHOP ATTENDEES ONLY (Foyer 260-071)

09:00 – 12:00 Workshops – morning session:

Room 040B	Room 040C	Case Room 3 055	Case Room 2 057
CCP4/AutoRickshaw workshop	Lipidic cubic phase workshop	CCDC/OLEX2 workshop	SBGrid workshop

12:00 – 12:30 Lunch - WORKSHOP ATTENDEES ONLY (Foyer 260-071)

12:30 – 3:00 Workshops – afternoon session:

Room 040B	Room 040C	Case Room 3 055	Case Room 2 057
CCP4/AutoRickshaw workshop	Lipidic cubic phase workshop	CCDC/OLEX2 workshop	Diffraction and spectroscopic methods at XFEL and synchrotron sources - workshop

2:00 – 3:00 Registration

3:00 – 3:30 Opening Ceremony Lecture Theatre 098

3:30 – 5:15 **General interest symposium:** Lecture Theatre 098
(Chair: Kurt Krause)

3:30 – 4:00	Anders Liljas	History of the crystallography as viewed through the lens of the Nobel Prize
4:00 – 4:20	Marc Storms	The role of Cryo-electron microscopy in structural biology after the “resolution revolution”
4:20 – 4:40	Piotr Sliz	X-ray Crystallography to Cryo-Electron Microscopy: Computing Infrastructure
4:40 – 5:10	George Phillips	The Future of Crystallography – or Not

5:15 – 6:00 **Keynote 1:** Yanli Wang Lecture Theatre 098
CRISPR-Cas Mediated Cleavage of Invading Nucleic Acids
(Chair: Mihwa Lee)

Keynote 2: Hiroshi Kitagawa Fisher & Paykel Appliances Auditorium
Toward dimensional crossover on conductive coordination networks
(Chair: Masaki Kawano)

6:00 – 7:00 **Plenary 1:** Susan Lea Fisher & Paykel Appliances Auditorium
Bacterial Protein Export Machines
(Chair: Jenny Martin)

7:00 – 8:30

Opening Night Mixer and Poster Session 1 (Foyer 260-101 & F&PAA Lobby)

MONDAY DECEMBER 3:

08:00 – 09:00 Registration

08:45 – 10:45 **MS#1: Membrane proteins:** Lecture Theatre OGGB3
(Chairs: Ruby Law, Satoshi Murakami)

8.45 – 9.10	Megan Maher	Structural snapshots of manganese uptake in <i>Streptococcus pneumoniae</i>
9.10 – 9.35	Kazuhiro Abe	Crystal structures of the gastric proton pump
9.35 – 10.00	Alisa Glukhova	Snapshots of GPCR-G protein complexes
10.00 – 10.15	Michael Parker	Structure-based drug discovery in Alzheimer's disease
10.15 – 10.30	Jason Busby	Chaperone-like encapsulation of insecticidal toxins
10.30 – 10.45	Karen Steffi Cheung Tung Shing	An insight in the assembly mechanism of the beta common cytokine receptors

08:45 – 10:45 **MS#2: Crystal engineering:** Lecture Theatre OGGB5
(Chair: Stuart Batten)

8.45 – 9.10	Edward Tiekink	The energies of non-standard intermolecular interactions are competitive with conventional hydrogen bonding
9.10 – 9.35	Hoi-Ri Moon	Exploration of Structural Transformations and Catalytic Selectivity in Tailored Flexible Metal-Organic Frameworks
9.35 – 9.55	Hidehiro Uekusa	Crystal Engineering of scented inclusion crystal and its sustained-release property
9.55 – 10.15	Joanna Stevens	Understanding polymorphism using hydrogen bond propensities
10.15 – 10.35	Ali Chahine	Selective carbon dioxide capture through adopting the backbone embedded amines into porous coordination polymers, 'the third approach'

08:45 – 10:45 **MS#3: Novel synchrotron and neutron applications:** Lecture Theatre OGGB4
(Chairs: Vanessa Peterson, Rachel Williamson)

8.45 – 9.10	Helen Brand	Shining a light on Martian processes using in situ neutron and synchrotron techniques
9.10 – 9.35	David Keen	Refining local structural disorder using combined synchrotron X-ray and spallation neutron total scattering/pair distribution functions
9.35 – 10.00	Dohyun Moon	Introduction of 2D-Supramolecular Crystallography Beamline (BL2D-SMC) at Pohang Light Source II in Korea
10.00 – 10.20	Connie Darmanin	XRD data from small aggregating crystals: Trials and tribulations
10.15 – 10.40	Shinji Kihara	Nanoplastics – protein interaction: A scattering study of the transition from soft to hard corona

10:45 – 11:15 Morning Tea (Foyer 260-071 & Foyer 260-088)

11:15 – 1:15 **MS#4. Applications of cryo-EM to structural biology:** Lecture Theatre OGGB3
(Chair: Mihnea Bostina)

11.15 – 11.35	Michael Landsberg	Cryo-EM structures of the pore-forming ABC toxin from <i>Yersinia entomophaga</i> provide insights into the dynamic structural rearrangement associated with membrane recognition
11.35 – 11.55	K R Vinothkumar	A novel metal-bound active site in a hydrolytic enzyme

11.55 – 12.15	Alok Mitra	A nanoscale injection mechanism: imaging the sheath contraction of the antifeeding prophage of <i>S. entomophila</i>
12.15 – 12.35	Atsushi Nakagawa	Hierarchical structure assembly mechanism of <i>Rice dwarf virus</i>
12.35 – 12.55	Cong Liu	The structural basis of reversible fibril involved in phase separation and neurodegenerative diseases
12.55 – 1.15	Chris Hill	Structural Basis for Substrate Translocation by the AAA ATPase Vps4

11:15 – 1:15 **MS#5. Solid state reactions and dynamics:** Lecture Theatre OGGB5
(Chairs: Chris Ling, Jun Harada)

11.15 – 11.40	Tomohiro Seki	Reversible phase transition between single crystals of luminescent gold complex
11.40 – 12.05	Matthew Rowles	<i>In situ</i> diffraction characterisation of hydrogen storage materials
12.05 – 12.30	Arnaud Grosjean	Elastic, plastic and creep deformation in one single crystal: structural investigations by micro focused X-ray diffraction
12.30 – 12.50	Takashi Ohhara	Temperature-induced intramolecular proton transfer in a novel polymorph of 2-(2'-hydroxyphenyl)benzimidazole crystal
12.50 – 1.10	Yumi Yakiyama	Structures and Properties of Porous Molecular Crystals Composed of Unique H-shape Molecules

11:15 – 1:15 **MS#6. Recent developments in crystal Growth:** Lecture Theatre OGGB4
(Chairs: Janet Newman, Barnali Chaudhuri)

11.15 – 11.40	Melissa Call	Analysing transmembrane helix interactions using lipid cubic phase crystallisation
11.40 – 12.05	Fasseli Coulibaly	Millennials microcrystals: wouldn't it be easier to stay home?
12.05 – 12.30	Robert Thorne	Solvent Behavior, Ice Formation, and Nanoconfinement in Protein Crystals: Implications for Cryo- and Variable-Temperature Crystallography
12.30 – 12.50	Rebecca Eno	Using mutants designed to alter crystal packing to determine mode of action of inhibitors for multiple herbicide resistance in weeds
12.50 – 1.10	Monika Budayova-Spano	Membrane-assisted protein crystallization

1:15 – 2:30 LUNCH (Foyer 260-071 & Foyer 260-088)
and Bruker Lunchtime workshop (Case Room 3 055)

2:30 – 4:30 **MS#7. Hybrid methods in structural Biology:** Lecture Theatre OGGB3
(Chairs: Grant Pearce, Sangho Lee)

2.30 – 2.55	Jose Rodriguez	Lattice nano-ripples revealed in peptide microcrystals by scanning electron nanodiffraction
2.55 – 3.20	Ji-Joon Song	Integrative Structural Investigation on Macromolecular Protein Complexes
3.20 – 3.45	Ruby Law	Structural Function Studies of Complement Component-9
3.45 – 4.00	Innokentij's Josts	Investigation of an ABC transporter MsbA in stealth carrier nanodiscs using small angle scattering techniques
4.00 – 4.15	Rhys Grinter	A tale of two proteases: Using X-rays to dissect the function of novel bacterial ferroprotein degradases
4.15 – 4.30	Stephanie Dawes	Molecular dynamics gives insights into TetR transcriptional regulator

2:30 – 4:30

MS#8. Structure and properties of functional materials:

Lecture Theatre OGGB5

(Chair: Hoi-Ri Moon)

2.30 – 2.55	Joanne Etheridge	Finding the atoms that matter in functional materials
2.55 – 3.20	Wonyoung Choe	Evolution of Form in Metal-Organic Frameworks
3.20 – 3.45	Dae-Woo Lim	Crystallographic understanding of proton conducting pathway with conducting medium confined in metal-organic frameworks
3.45 – 4.05	Pramod Halappa	Effect of local structure variation on Photo-catalytic Organic Transformation activity of Iso-structural PbW _{1-x} MoxO ₄ Nano-solid Solutions
4.05 – 4.25	Pierre Naeyaert	The Effect of K-doping on the Performance of P2-type Na-ion Battery Cathode Materials

2:30 – 4:30

MS#9. XFELs and serial crystallography:

Lecture Theatre OGGB4

(Chairs: Connie Darmanin, Hiroshi Sugimoto)

2.30 – 2.55	Minoru Kubo	Time-Resolved XFEL Crystallography for Capturing Reaction Intermediates of Respiratory Metalloenzymes
2.55 – 3.20	Richard Bean	SPB/SFX: First Experimental Results and Future Developments
3.20 – 3.45	Clyde Smith	New opportunities for structural biology research at LCLS and SSRL
3.45 – 4.00	Takashi Kumasaka	Development of fixed-target serial crystallography at room temperature in SPring-8
4.00 – 4.15	Andrew Martin	Fluctuation x-ray scattering: measuring the statistics of local 3D structure of amorphous materials, liquids and nanocrystals
4.15 – 4.30	Susannah Holmes	The effect of consecutive X-ray pulses on a single crystal at the European XFEL

4:30 – 5:00

Afternoon Tea (Foyer 260-071 & Foyer 260-088)

5:00 – 6:00

Plenary 2:

Cameron Kepert

Fisher & Paykel Appliances Auditorium

Adventures in Diffraction: Probing Dynamic Processes within Molecular Framework Materials

(Chair: Shane Telfer)

6:00 – 7:45

Networking Mixer and Poster Session 2 (Foyer 260-101 & F&PAA Lobby)*Sponsored by School of Biomedical Sciences, University of Otago*

TUESDAY DECEMBER 4:

08:00 – 09:00 Registration

8:45 – 9:30 **SCANZ Mathieson Lecture:** Lecture Theatre 098
 Suzanne Neville
 Molecular Switching Framework Materials
 (Chair: Chris Sumby)

9:30 – 10:15 **Keynote 3:** Richard Neutze Lecture Theatre OGGB3
 Time-resolved diffraction experiments at X-ray free electron lasers
 reveal ultrafast structural changes in photosynthesis
 (Chair: Richard Kingston)

Keynote 4: Deanna D'Alesandro Lecture Theatre OGGB4
 Harnessing Electroactivity in Coordination Frameworks
 (Chair: Edward Tiekink)

10:15 – 10:45 Morning Tea (Foyer 260-071 & Foyer 260-088)

10:45 – 12:45 **MS#10. Disease-related proteins:** Lecture Theatre OGGB3
 (Chairs: Bostjan Kobe, Hanna Yuan)

10.45 – 11.10	Emily Parker	Twisting tales and pKa pathways in key biosynthetic enzymes
11.10 – 11.35	Yonggui Gao	Antibacterial drug resistance through ribosome protection ATP-binding cassette protein
11.35 – 11.50	Ruchi Anand	Using Structural Biology as a tool to Decipher Origins of Antibiotic Resistance
11.50 – 12.05	J Sivaraman	Structural basis for the function of ScpC, a virulence protease from <i>Streptococcus pyogenes</i>
12.05 – 12.20	Luke Guddat	Targeting branched chain amino acid biosynthesis for herbicides and antifungals
12.20 – 12.45	Nei-Li Chan	Structural Insights into the Gating of DNA Passage by the Topoisomerase II DNA-Gate

10:45 – 12:45 **MS#11. MOFs and hybrid materials:** Lecture Theatre OGGB5
 (Chairs: Lauren Macreadie, J J Vittal)

10.45 – 11.10	Shane Telfer	Pore Programming in Multicomponent Metal-Organic Frameworks
11.10 – 11.35	Shiho Sairenji	Determination of the Absolute Configuration of Compounds Bearing Chiral Quaternary Carbon Centers Using the Crystalline Sponge Method
11.35 – 12.00	Shim Sung Lee	Pillar[5]arene as a new member in MOFs and hybrid materials
12.00 – 12.15	Stuart Batten	Alkylamine Coordination Polymers for CO ₂ Capture
12.15 – 12.30	Wei-Yin Sun	Metal-organic frameworks with chelating multiamine ligands: synthesis and properties
12.30 – 12.45	Winnie Cao	Crystal engineering of chiral coordination polymers with amino acid derived ligands

10:45 – 12:45 **MS#12. Advanced methods in crystallography, electron diffraction and cryo-EM:** Lecture Theatre OGGB4
 (Chair: Dominika Elmlund)

10.45 – 11.10	Hans Elmlund	Algorithms for real-time unsupervised cryo-EM structure determination
11.10 – 11.25	Wei Ding	IPCAS: A Pipeline from Phasing to Model Building and Refinement for X-ray Diffraction Data and Cryo-EM Density Map
11.25 – 11.40	Pavel Afonine	New Phenix tools for validation of cryo-EM maps and models
11.40 – 12.05	Yungwon Park	Multi-dimensional liquid phase TEM for studying colloidal nanoparticles

12.05 – 12.20	Jianbo Wang	Atomistic and Real-time Structural Characterization in Metal Oxides
12.20 – 12.45	Tamir Gonen	MicroED: conception, practice and future opportunities

12:45 – 2:00 LUNCH (Foyer 260-071 & Foyer 260-088)
Thermo Fisher Scientific Lunchtime workshop (Case Room 3 055)
1:00 – 2:00 SCANZ Business Meeting (Case Room 2 057)

2:00 – 4:00 **MS#13. Hot structures-biology:** Lecture Theatre OGGB3
(Chairs: Peter Czabotar, Ruchi Anand)

2.00 – 2.25	Emily Furlong	Studies of the trimeric disulfide isomerase PmScsC and its redox partner PmScsB α
2.25 – 2.50	Kayarat Saikrishnan	Structure-based mechanism of nucleotide-dependent restriction endonuclease
2.50 – 3.15	Toshiharu Suzuki	Static and dynamic X-ray crystallographic analyses of reaction intermediate states of mammalian F1-ATPase to reveal the physical power generation mechanism
3.15 – 3.30	Gayathri Pananghat	Mechanism of allosteric activation of a prokaryotic small Ras-like GTPase by an asymmetric dimer interaction
3.30 – 3.45	Andrew McCarthy	Crystal structure of METTL16, an RNA m6A writer that is essential for mouse embryonic development
3.45 – 4.00	Bostjan Kobe	Structural basis of NAD ⁺ cleavage activity by mammalian and plant TIR domains

2:00 – 4:00 **MS#14. Microcrystalline materials, ceramics and minerals:** Lecture Theatre OGGB5
(Chair: Tilo Soehnel)

2.00 – 2.25	Timothy White	Structural Flexibility and Tunable Functionality
2.25 – 2.50	Maxim Avdeev	Combining X-ray and neutron diffraction and modelling for better understanding advanced materials
2.50 – 3.15	Kotaro Fujii	Origin of the high oxide-ion conductivity in the apatite-type lanthanum silicates
3.15 – 3.30	Helen Maynard-Casely	The many phases of acrylonitrile
3.30 – 3.45	Jun Harada	Development of plastic/ferroelectric ionic molecular crystals
3.45 – 4.00	Chris Howard	An algebraic approach to cooperative rotations in networks of interconnected rigid units

2:00 – 4:00 **MS#15. Database developments, validation & data mining:** Lecture Theatre OGGB4
(Chairs: Genji Kurisu, Amy Sarjeant)

2.00 – 2.15	James Hester	What is a dataset?
2.15 – 2.40	Janet Newman	Data for Crystallisation – Answers are in the distance
2.40 – 2.55	Matthew Lightfoot	The Cambridge Structural Database – Developments in deposition and access
2.55 – 3.20	Stephen Burley	Ligand Validation for the Protein Data Bank
3.20 – 3.35	Takeshi Kawabata	Databases and Web services from PDBe for Electron Microscopy
3.35 – 4.00	Brian McMahon	The element of trust: validating and valuing crystallographic data

4:00 – 4:30 Afternoon Tea (Foyer 260-071 & Foyer 260-088)

4:30 – 5:30 **Plenary 3 – PUBLIC LECTURE:** Fisher & Paykel Appliances Auditorium
David Eisenberg

Amyloid Fibrils in Health and Disease

(Chair: Ted Baker)

Sponsored by School of Biological Sciences, University of Auckland

7:00 – 11:30

Rigaku Conference Dinner – Auckland War Memorial Museum

WEDNESDAY DECEMBER 5:

08:00 – 09:00 Registration

8:45 – 9:30 **Keynote 5:** Catherine Day Lecture Theatre OGGB3
Building chains: regulation of ubiquitin transfer by E3 ligases
(Chair: Jodie Johnston)
Sponsored by Maurice Wilkins Centre

Keynote 6: Ayana Sato-Tomita Lecture Theatre OGGB4
Capturing a protein reaction triggered by laser photolysis in crystals
(Chair: Tom Caradoc-Davies)

9:30 – 10:15 **SCANZ Bragg Lecture:** Lecture Theatre 098
Mitchell Guss
My life in crystallography
(Chair: David Aragao)

10:15 – 10:45 Morning Tea (Foyer 260-071 & Foyer 260-088)

10:45 – 12:45 **MS#16. Macromolecular complexes & assemblies:** Lecture Theatre OGGB3
(Chairs: David Goldstone, Xiao-Dong Su)

10.45 – 11.10	Zihe Rao	Structures of the Herpes simplex virus type 2 B-capsid and C-capsid with capsid-vertex-specific component
11.10 – 11.35	Satoshi Murakami	Structure and function of tripartite drug efflux transporters in Gram-negative bacteria
11.35 – 12.00	Ruiming Xu	Structural basis for regulation of histone acetylation
12.00 – 12.15	Peter Mace	A bidentate Polycomb Repressive-Deubiquitinase complex is required for efficient activity on nucleosomes
12.15 – 12.30	Mirosław Cygler	Structure and Dynamics of the Core Fe/S Cluster Assembly Complex
12.30 – 12.45	Gabrielle Watson	Structural basis of CD96 immune receptor recognition of nectin-like protein-5 (CD155)

10:45 – 12:45 **MS#17. Hot structures – chemistry:** Lecture Theatre OGGB5
(Chairs: Chien Ing (Ally) Yeo, Geoff Jameson)

10.45 – 11.10	Jagadese Vittal	Engineering of Photoreactive and Photosensitive Crystals
11.10 – 11.35	Masaki Kawano	Kinetic Assembly of Porous Coordination Networks
11.35 – 12.00	Elodie Rousset	Structure determination of twinned and poorly diffracting crystals suffering radiation damage using the MX beamlines at the Australian Synchrotron
12.00 – 12.15	Lauren Macreadie	Mixed-metal MOFs comprised of phenanthroline ligands with carboxylate functionalities
12.15 – 12.30	Tan Yee Seng	Crystal transformation and meta-stable forms of a tetramorphic one-dimensional coordination polymer of cadmium dithiophosphate with a bipyridine linker
12.30 – 12.45	Alison Edwards	On model phasing for Thorium (and other heavy element) clusters – getting the hydrides right

10:45 – 12:45 **MS#18. Novel applications of Crystallography:** Lecture Theatre OGGB4

(Chairs: Helen Maynard-Casely, Huijeong Hwang).

10.45 – 11.10	Stephen Moggach	The effect of pressure, temperature and gas uptake within fullerene stabilised phthalocyanine nanoporous molecular crystals
11.10 – 11.30	Tomoki Fujita	Solvothermal reactor for in-situ synchrotron radiation powder diffraction at SPring-8 BL02B2 for quantitative design for nanoparticle
11.30 – 11.50	Takeshi Matsukawa	Investigation of crystal structure of reduced ceria under hydrogen by powder neutron diffraction
11.50 – 12.15	Huijeong Hwang	Dynamic compression at Pohang X-ray Free Electron Laser Facility (PAL-XFEL)
12.15 – 12.35	Liang Li	Hexamethylbenzene: Ant or Elephant? A 3D Bendable Crystal with Giant Power Output Capability

12:45 – 2:00 LUNCH (Foyer 260-071 & Foyer 260-088)

1:00 – 2:00 AsCA Council Meeting (Case Room 3 055)

2:00 – 4:00 **Rising Star Symposium** Lecture Theatre 098
(Chairs: Alice Vrielink, Pinak Chakrabati)

2:00 – 2:20	Sanchari Banerjee	Microcrystallography of heterogenous in vivo-grown protein crystals from the viviparous cockroach <i>Diploptera punctata</i>
2:20 – 2:40	Yuka Deguchi	Charge density study of diamond at 800K using data correction for weak intensities
2:40 – 3:00	Matthias Fellner	Lactate racemization, a story of so much more than just a nickel
3:00 – 3:20	M. Mozzam Naseer	Noncovalent Carbon Bonding: Is it a σ -hole interaction of broad implications?
3:20 – 3:40	Kate Smith	Structural basis for importin alpha 3 specificity of W proteins in Hendra and Nipah viruses
3:40 – 4:00	Katrina Zenere	A Spin Crossover Framework That Does It All

4:00 – 4:30 Afternoon Tea (Foyer 260-071 & Foyer 260-088)

4:30 - 5:30 **Plenary 4 - SCANZ 1987 Lecture:** Lecture Theatre 098
Amy Rosenzweig
(Chair: Helen Maynard-Casely)

5:30 – 6:00 **Closing Ceremony** Lecture Theatre 098