## **Monday 21 August**

## Pre-Congress Workshops

7.00am - 3.00pm				Registrat	ion Open								
	Room: 205	Room: 206	Room: 208	Room: 209	Room: 214	Room: 215	Room: 216	Room: 217					
8.00am - 1.00pm	Next-generation atomistic- level structural modeling using combined powder and single-crystal scattering data Session 1	CIF Dictionary Workshop Session 1	A practical approach to synchrotron experiments	Online and free tools for crystallographic symmetry handling and visualization Session 1	Quantum crystallography workshop Session 1	UMD: Melts and Fluids from Ab Initio Molecular Dynamics Simulations Session 1	APEX4 How to Start?  Sponsored by Bruker	CCP4/CCP-EM Workshop Session 1					
1.00pm - 2.00pm	Break												
	Room: 205	Room: 206	Room: 208	Room: 209	Room: 214	Room: 215	Room: 216	Room: 217					
2.00pm - 6.00pm	Next-generation atomistic- level structural modeling using combined powder and single-crystal scattering data Session 2	CIF Dictionary Workshop Session 2	Advances in macromolecule microcrystallography	Online and free tools for crystallographic symmetry handling and visualization Session 2	Quantum crystallography workshop Session 2	UMD: Melts and Fluids from Ab Initio Molecular Dynamics Simulations Session 2	<b>OLEX2</b> Session 1	CCP4/CCP-EM Workshop Session 2					

## **Tuesday 22 August**

# Pre-Congress Workshops and Congress Opening

	I												
7.00am - 6.30pm					Registrat	ion Open							
	Room: 205	Room: 206	Room: 208	Room: 209	Room: 214	Room: 215	Room: 216	Room: 217	Room: 219	Room: 220			
8.00am - 12.00pm	Raw diffraction data reuse: the good, the bad and the challenging Session 1	RMCProfile: "Big-box" modelling for total scattering data Session 1	UMD: Melts and Fluids from Ab Initio Molecular Dynamics Simulations Session 3	Online and free tools for crystallographic symmetry handling and visualization Session 3	Quantum crystallography workshop Session 3	Workshop on X-ray Absorption Fine Structure Session 1	APEX4 Advanced Features Workshop Sponsored by Bruker	CCP4/CCP-EM Workshop Session 3	Crystallographic and cryo-EM structure solution with Phenix Session 1	Using the CSD to go from data to discoveries Session 1			
12.00pm - 1.00pm	Break												
	Room: 205	Room: 206	Room: 208	Room: 209	Room: 214	Room: 215	Room: 216	Room: 217	Room: 219	Room: 220			
1.00pm - 4.00pm	Raw diffraction data reuse: the good, the bad and the challenging Session 2	RMCProfile: "Big-box" modelling for total scattering data Session 2	Non-Ambient X-ray Diffraction (NA-XRD) of Powders and Thin Films	75th Anniversary of IUCr - refresh of vision and values	Understanding viscosity using RheoSAXS	Workshop on X-ray Absorption Fine Structure Session 2	<b>OLEX2</b> Session 2	CCP4/CCP-EM Workshop Session 4	Crystallographic and cryo-EM structure solution with Phenix Session 2	Using the CSD to go from data to discoveries Session 2			
4.30pm - 7.00pm	IUCr 2023 Official Opening Ceremony & 13th Ewald Prize Lecture by Prof Wayne A. Hendrickson												
7.00pm - 9.00pm	Congress Welcome Reception IUCr 2023 Exhibition												

## Wednesday 23 August

Day 2

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8.00am - 7.00pm							Registration Open						
	Room: 203/4	Room: 205	Room: 207	Room: 208	Room: 209	Room: 210/11	Room: 212/13	Room: 214	Room: 215	Room: 216	Room: 217	Room: 219	Room: 220
9.00am - 9.50am	Keynote 1 Dr Thomas Terwilliger Commission on Biological Macromolecules	Child Care				Chair: Akiko Sekine  Keynote 2  Prof Masako Kato  Commission for Structural  Chemistry	Chair: Koen Janssens  Keynote 3  Dr Silvie Švarcová  Commission on  Crystallography in Art and  Cultural Heritage	Software Fayre					
9.50am - 10.20am							Morning Tea						•
	Room: 203/4	Room: 205	Room: 207	Room: 208	Room: 209	Room: 210/11	Room: 212/13	Room: 214	Room: 215	Room: 216	Room: 217	Room: 219	Room: 220
	Chair Jan Ilavsky					Chair: Mauro Gemmi	Chair: Geetha Balakrishna						
10.20am - 11.10am	Keynote 4 Prof Michelle Calabrese Commission for Small-Angle Scattering  Posters					Keynote 5 Prof Joanne Etheridge Commission on Electron Crystallography	Keynote 6 Dr Elias Vlieg Commission on Crystal Growth and Characterization of Materials	Software Fayre					
11.10am - 12.10pm					Posters							Posters	
12.10pm - 1.10pm			Lu	nch			DECTRIS PILATUS4 Product Launch over free lunch Sponsored by DECTRIS  12.20pm - 1.05pm	Li	unch	Closed meeting of the Commission on Diffraction of Microstructure Imaging (CDMI) 11.10am - 1.00pm	Materials over free lunch Sponsored by Eldico	Lunch	Closed meeting of the Commission for Crystallographic Teaching 12:00pm - 1.00pm
	Room: 203/4	Room: 203/4 Room: 205 Room: 207 Room: 208 Room: 209 Room						Room: 214	Room: 215	Room: 216	12.20pm - 1.05pm Room: 217	Room: 219	Room: 220
	Chairs: Ewa Grzanka	Chairs: Dmitry Sebastián Session: Crystal Stru	Chairs: Dmitry Golberg & Sebastián Suarez	Chairs: Alexander Wlodawer	Chairs: Tristan Croll	NSOIN: 229/22	Room: 212/13  Chairs: Karena Chapman & Poul Norby	1100.111 224	NOUTI. 223	Chairs: Victor Streltsov	Chairs: Holger Klein & Stéphanie Kodjikian	Chairs: Lauren Macreadie & Nils Nöthling	Chairs: Joe Paddison
	Session: A041 Crystal Growth for Emerging technologies - from Medicine to Semiconductors		Session: A040 Crystal Structure of Functional Materials	Session: A013 Rapid Response Toward Biomedical Threats	Session: A020 Modern Statistical Tools and Computational Methods in Structure Determination		Session: A076 In-situ Studies of Materials Synthesis and Crystal Growth			Session: A112 X-ray Imaging and Spectroscopy in Life Sciences	Session: A036 Combining Electron and X- ray Crystallography for Structure Characterization	Session: A093 Nucleation and Crystal Growth	Session: A055 Diffuse Scattering Analysis of Short Range Crystal and Magnetic Order
	#345 - Dr Aurelio Borzì Contributed talk 1		#172 - Prof Joke Hadermann Contributed talk 1	#502 - Dr Mihwa Lee Contributed talk 1	#811 - Dr Oleg Sobolev Contributed talk 1		#437 - Dr Kevin Stone Contributed talk 1		Journal Editors Meeting 13:00 - 15:00	#875 - Dr Chanh Tran Contributed talk 1	#566 - Mrs Sepideh Rahimi Contributed talk 1	#273 - Miss Alexandra Longcake Contributed talk 1	#1188 - Dr Ella Mara Schmidt Contributed talk 1
1.10pm - 3.30pm	#1573 - Prof Xiaodong Su Contributed talk 2	Child Care	#584 - Dr Semën Gorfman Contributed talk 2	#358 - Dr Bronte Johnstone Contributed talk 2	#585 - A/Prof Anders Østergaard Madsen Contributed talk 2		#234 - Miss Elizabeth Galtry Contributed talk 2	Software Fayre	All IUCr Journal editors and co-editors welcome	#722 - Dr Joanna Slawek Contributed talk 2	#56 - Prof Josef Simbrunner Contributed talk 2	#1953 - Dr Kasun Athukorala Arachchige Contributed talk 2	#1740 - Miss Manisha Islan Contributed talk 2
	<b>Dr Valeria Murgulov</b> Invited Speaker 1		A/Prof Laure Bourgeois Invited Speaker 1	Prof Zihe Rao Invited Speaker 1	<b>Dr Richard Kingston</b> <i>Invited Speaker 1</i>		<b>Dr Sylvie Le Floch</b> Invited Speaker 1			Miss Abbey Telfer Invited Speaker 1	<b>Dr Kiyofumi Takaba</b> Invited Speaker 1	<b>Dr Martin Adam</b> Invited Speaker 1	<b>Dr Pascal Manuel</b> Invited Speaker 1
	#1599 - Dr Andrew Stevenson Contributed talk 3		#1792 - Ms Erica Cordero Oyonarte Contributed talk 3	#1301 - Prof Megan Maher Contributed talk 3	#117 - Prof Randy Read Contributed talk 3		#159 - Dr Hidetaka Kasai Contributed talk 3			Contributed talk 3	#1128 - Dr Oleg Prymak Contributed talk 3	#609 - Ms Yui Wakasa Contributed talk 3	#934 - Ms Yevheniia Kholina Contributed talk 3
	#1727 - Dr Robert Czernecki Contributed talk 4		Contributed talk 4	#100 - Prof Ramaswamy Subramanian Contributed talk 4	Contributed talk 4		#1396 - Prof Yoshiyuki Inaguma Contributed talk 4			Contributed talk 4	#259 - Ms Romy Poppe Contributed talk 4	#81 - Miss Jessica Metherall Contributed talk 4	#576 - Prof Andrew Goodwin Contributed talk 4
	<b>Dr Dorota Pawlak</b> Invited Speaker 2		Prof Simon P. Ringer Invited Speaker 2	Prof Wladek Minor Invited Speaker 2	<b>Dr Tom Burnley</b> Invited Speaker 2		<b>Dr. Fan Zhang</b> Invited Speaker 2			<b>Dr Saša Bajt</b> Invited Speaker 2	Prof. Karla Balzuweit Invited Speaker 2	<b>Dr Helen Brand</b> Invited Speaker 2	<b>Dr Benjamin Frandsen</b> Invited Speaker 2
							Afternoon Tea						
3.30pm - 4.00pm							/ intermoon red						

	Chairs: Wladek Minor & Emily Parker		Chairs: Alexander Grishaev & Dina Schneidman	Chairs: Yongjae Lee & Helen Brand	Chairs: John Claridge & Inbal Tuvi-Arad (Julia Conteras Garcia)			Chairs: Loes Kroon- Batenburg & James Hester	Chairs: Leo Chavas & Fasseli Coulibaly	Chairs: Samuel Tetteh & Suzanna Ward	Chairs: Ben Frandsen & Oksana Zaharko
	Session: A007 Structural Biology in the Fight Against Infectious Diseases		Session: A090 Biomolecular SAS and Integrative methods: Standards and Validation	Session: A050 Complex Structures of Minerals and Inorganic Materials	Session: A027 Teaching Crystallographic Symmetry for Materials Science			Session: A118 Raw Diffraction Data Reuse: Warts and All	Session: A111 In vivo crystallography and synchrotron radiation	Session: A104 Structural databases in materials development	Session: A062 Geometrically-frustrated Magnetism
	#580 - Prof Begona Heras Contributed talk 1		#1756 - Mr Heidar Koning Contributed talk 1	#213 - Dr Jai Prakash Contributed talk 1	#721 - Prof Inbal Tuvi-Arad Contributed talk 1			#321 - Prof Simon Coles Contributed talk 1	#594 - Dr Dominik Oberthuer Contributed talk 1	#1526 - Dr Patrice Kenfack T. Contributed talk 1	#125 - Dr Ovidiu Garlea Contributed talk 1
4.00pm - 6.30pm	#278 -Prof Stephanie Gras Contributed talk 2	Child Care	#1754 - Dr Joseph Kline Contributed talk 2	#1176 - Dr Chloe Fuller Contributed talk 2	#1609 - Dr Lauro Bucio Contributed talk 2		Closed Meeting for the	#717 - Dr Oleksandr Yefanov Contributed talk 2	#488 - Dr Kunio Hirata Contributed talk 2	#735 - Dr Olga Grineva Contributed talk 2	#904 - Van Duijn Contributed talk 2
	Prof Ian Wilson Invited Speaker 1		Prof Jill Trewhella Invited Speaker 1	<b>Dr Matt Tucker</b> Invited Speaker 1	#591 - Prof Joke Hadermann Invited Speaker 1	Software Fayre	Scattering 4:00pm - 5:00pm	Dr Gerard Bricogne Invited Speaker 1	Prof Petra Fromme Invited Speaker 1	Dr Tom Blanton Invited Speaker 1	Dr Joseph Paddison Invited Speaker 1
	#1787 - Prof Maria Cristina Nonato Contributed talk 3	_	#1612 - Dr Andrew Whitten Contributed talk 3	Contributed talk 3	Dr Ilaria Gimondi Invited Speaker 2			#412 - Dr James Hester Contributed talk 3	#739 - Mrs J. Mia Lahey- Rudolph Contributed talk 3	#1474 - Prof Vitaliy Kurlin Contributed talk 3	#684 - Dr Eamonn Connolly Contributed talk 3
	#1764 - Prof Haitao Yang Contributed talk 4		#1170 - Prof U-Ser Jeng Contributed talk 4	#275 - Mr Seiya Takahashi Contributed talk 4				Dr Malcolm Guthrie Invited Speaker 2	#1763 - Prof Lars Redecke Contributed talk 4	Contributed talk 4	#810 - A/Prof Mirela Dragomir Contributed talk 4
	Dr Andrzej Joachimiak Invited Speaker 2		Dr Brinda Vallat Invited Speaker 2	Dr Daniel Chaney Invited Speaker 2				#784 - Dr Soorya Kabekkodu Contributed talk 4	Takafumi UENO Invited Speaker 2	Julia Gasol Cardona Invited Speaker 2	A/Prof Kirrily Rule Invited Speaker 2
6.30pm - 7.00pm				<b>Dr Oliver Perez</b> Invited Speaker 3							
											Room: 219/220
7.30pm - 10.30pm											General Assembly 1 7.30pm - 10.30pm

### **Thursday 24 August**

						Day 3							
8.30am - 4.30pm						Registration Open							
	Room: 203	Room: 204	Room: 205	Room: 210	Room: 211	Room: 212	Room: 213	Room: 214	Room: 215	Room: 219	Room: 220		
0.00 0.50	Chair: Atsus	hi Nakagawa		Chair: S	hilie Pan	Chair: Ma	ax Avdeev						
9.00am - 9.50am	Keyr Dr Alexando Commission on Biolo		Child Care	Keyn Prof Gra Commission on St.			ote 9 a Zaharko agnetic Structures	Software Fayre					
9.50am - 10.20am						Morning Tea							
	Room: 203	Room: 204	Room: 205	Room: 210	Room: 211	Room: 212	Room: 213	Room: 214	Room: 215	Room: 219	Room: 220		
40.30 44.40	Chair: Giulia	na Aquilanti		Chair Christi	ian Lehmann	Chair: Joh	n Daniels						
10.20am - 11.10am	Keyn Dr Danie Commission on X-ray Al		Child Care	Keyno Prof Angel N Commission on Quan		Keyno Dr Hele Commission on Crystallograph		Software Fayre					
11.10am - 12.10pm		Posters											
12.10pm - 1.10pm	·			Latest innovations from XRD to nanoparticles analysis (over free lunch & beer) Sponsored by Malvern Panalytical  12.20pm - 1.05pm		Latest innovations from Rigaku Oxford Diffraction over free lunch Sponsored by Rigaku 12.20pm - 1.05pm	Lunch	Closed meeting of the Commission on XAFS 12:00pm - 1.00pm	IUCr Journals Open Meeting including referee workshop 12:00pm - 1:00pm All past and future authors, editors and reviewers welcome	Lunch	Closed meeting of the Commission on Magnetic Structures 11:15am - 1.00pm		
	Room: 203	Room: 204	Room: 205	Room: 210	Room: 211	Room: 212	Room: 213	Room: 214	Room: 215	Room: 219	Room: 220		
	Chairs: Melissa Call & Catherine Drennan	Chairs: Silvie Švarcová & Catherine Dejoie		Chairs: Hoi Ri Moon	Chairs: Branton Campbell & J. Paul Attfield	Chairs: Uwe Müller	Chairs: Darren Pagan			Chairs: Randi Holmestad & Ya-Sen Sun	Chairs: Dharmalingam Prabhakaran		
	<b>Session: A017a</b> Enzyme Mechanisms and Regulation	Session: A001 and A002 Crystallographic Approaches to Study Cultural Heritage and Artists Materials and their Spontaneous Degradation		Session: A098 Postsynthetic modification of crystals	<b>Session: A077</b> Phase Transitions	Session: A021 Computing in Fragment Screening	Session: A028 Insights from 3D Diffraction Microstructural Imaging of insitu Deformation of Engineering Alloys			Session: A035 Multimodal approaches to interfaces, defects and thin films	Chairs: Silvie Švarcová		
1.10pm - 3.30pm	#1400 - Dr Alhonsa Benjdia Contributed talk 1	#521 - Prof. Koen Janssens Contributed talk 1	<b>a</b>	#379 - A/Prof Tatsuhiro Kojima Cancelled Contributed talk 1	#477 - Prof Chris Ling Contributed talk 1	#470 - Dr Kate Smith Contributed talk 1	#1413 - Mr Felix Frankus Contributed talk 1			#235 - Dr Celine Durniak Contributed talk 1	#683 - Ms. Pragati Pherwani Contributed talk 1		
	#467 - Prof Atsushi Nakagawa Contributed talk 2	#797 - Dr Marek Kotrlý Contributed talk 2	Child Care	#507 - Dr Pavel Usov Contributed talk 2	#313 - Prof Rene Guinebretiere Contributed talk 2	#1123 - Dr Alessandro Caputo Contributed talk 2	#1685 - Mr Sina Borgi Contributed talk 2	Software Fayre		#963 - Prof Louisa Meshi Contributed talk 2	#493 - Prof Sundaresan Athinarayanan Contributed talk 2		
	Prof Emily Parker Invited Speaker 1	Prof Gilberto Artoli Invited Speaker 1		Prof Natalia B. Shustova Invited Speaker 1	<b>Dr Wei-Tin Chen</b> Invited Speaker 1	<b>Dr May Sharpe</b> Invited Speaker 1	Prof Alicia Esther Ares Invited Speaker 1			<b>Jian-Min Zuo</b> Invited Speaker 1	Dr Ekaterina Pomjakushina Invited Speaker 1		
	#1532 - Prof Luke Guddat Contributed talk 3	#708 - Prof Takashi Kamiyama Contributed talk 3		#331 - Dr Thomas Roseveare Contributed talk 3	<b>#1197 - Hiroshi Abe</b> Contributed talk 3	#1735 - Dr Rachel Williamson Contributed talk 3	#1183 - Mr James Ball Contributed talk 3			#308 - Dr Chun-Ming Wu Contributed talk 3	#800 - Dr Dharmalingam Prabhakaran Contributed talk 3		

	#1554 - Prof Tam Greaves Contributed talk 4	#816 - Prof. Nourredine Benali-cherif Contributed talk 4		#58 - Prof Kana Sureshan Contributed talk 4	#544 - Dr Christopher Ridley Contributed talk 4	<b>Dr Tobias Krojer</b> Invited Speaker 2	Contributed talk 4			#1656 - Dr Wei Chao Contributed talk 4	#2091 - Mr Taikang Chen Contributed talk 4
	Prof Shekhar Mande Invited Speaker 2	Dr Filomena Salvemini Invited Speaker 2		Prof. Zhenjie Zhang Invited Speaker 2	A/Prof Emma McCabe Invited Speaker 2	#3060 - Mrs Tatjana Barthel Contributed talk 4	Dr Alberto Leonardi Invited Speaker 2			<b>Prof Xiaodong Zou</b> Invited Speaker 2	Prof Devashibhai Adroja Invited Speaker 2
3:30pm - 3:50pm					#14872 - Dr Alexei Bosak Contributed talk 5						
3.30pm - 4.00pm						Afternoon Tea	-				
	Room: 203	Room: 204	Room: 205	Room: 210	Room: 211	Room: 212	Room: 213	Room: 214	Room: 215	Room: 219	Room: 220
,	Chairs: Melissa Call & Catherine Drennan	Chairs: Stephen Skinner		Chairs: Lorraine Malaspina & Helen Maynard-Casely	Chairs: Matthew R. Rowles	Chairs: Ryuji Tamura	Chairs: Peter Spackman			Chairs: Daisuke Hashizume & Simon Coles	Chairs: Fan Zhang
	Session: A017b Enzyme Mechanisms and Regulation	Session: A049 Crystallography of Solid-state Ionic Conductors	Child Care	Session: A097 Applications of Neutron Diffraction for Chemical Crystallography	Session: A080 Industrial and Engineering Powder Diffraction	Session: A056 Magnetic Order in Aperiodic Systems	Session: A063 Crystal Structure Prediction			Session: A084 Structural chemistry (r) evolution by quantum crystallography	Session: A091 Advanced Characterization of Additive Manufacturing usin Synchrotron and Neutron Scattering Methods
	#921 - Ms Alison Biester Contributed talk 1	#1629 - Dr Masatsugu Yoshimoto Contributed talk 1		#491 - Dr Takashi Ohhara Contributed talk 1	#802 - Dr Tom Blanton Invited Speaker 1	#564 - A/Prof Karen Friese Contributed talk 1	#663 - Dr Lily Hunnisett Contributed talk 1			#1192 - Dr Jozef Kozisek Contributed talk 1	#1430 - Dr Tilman Donath Contributed talk 1
4.00pm - 6.30pm	#1662 - Dr Armin Wagner Contributed talk 2	#175 - Prof Stephen Hull Contributed talk 2		#1608 - Dr Keishiro Yamashita Contributed talk 2	#1346 - Prof Miguel A.G. Aranda Contributed talk 2	#1697 - Dr Shintaro Suzuki Contributed talk 2	#602 - Dr Mihails Arhangelskis Contributed talk 2	Software Fayre		#1576 - A/Prof Sajesh P. Thomas Contributed talk 2	#1707 - Dr Alberto Leonard Contributed talk 2
	<b>Dr Wei Shen Aik</b> Invited Speaker 1	Dr Josie Auckett Invited Speaker 1		<b>Prof. David Turner</b> <i>Invited Speaker 1</i>	Prof James A. Kaduk Invited Speaker 2	<b>Dr. Farid Labib</b> <i>Invited Speaker 1</i>	<b>Dr Johannes Hoja</b> <i>Invited Speaker 1</i>			Prof Kunihisa Sugimoto Invited Speaker 1	<b>Dr Jan Ilavsky</b> Invited Speaker 1
	#1636 - A/Prof Christopher Squire Contributed talk 3	#402 - Dr Yajun Yue Contributed talk 3		#716 - Dr Alison Edwards Contributed talk 3	#6 - Dr Huan Doan Contributed talk 3	#520 - Dr John Claridge Contributed talk 3	#926 - A/Prof Leopoldo Suescun Contributed talk 3			#319 - Prof Horst Puschmann Contributed talk 3	#613 - Dr Olga Narygina Contributed talk 3
	#438 - Mr Jisub Hwang Contributed talk 4	#763 - Prof Paul Henry Contributed talk 4		#197 - Dr Matthias Gutmann Contributed talk 4	Prof Vanessa Peterson Invited Speaker 3	#1163 - Dr Yuji Muro Contributed talk 4	#1714 - Mrs Maria Fedyaeva Contributed talk 4			#524 - Ms Lavanya Kumar Contributed talk 4	#1405 - Dr Suresh Koppoju Contributed talk 4
	Prof Samar Hasnain Invited Speaker 2	<b>Dr Kotaro Fuji</b> Invited Speaker 2		Dr. Amber Thompson Invited Speaker 2		<b>Dr T.J. Sato</b> Invited Speaker 2	Dr Jack Yang Invited Speaker 2			Dr Lorraine Andrade Malaspina Invited Speaker 2	#1322 - Dr Yu-Sheng Chen Contributed talk 5
											Room: 219/220
7.30pm - 10.30pm											General Assembly 2 7.30pm - 10.30pm

### Friday 25 August

8.30am - 7.00pm						Registration Open					
	Room: 203	Room: 204	Room: 205	Room: 210	Room: 211	Room: 212	Room: 213	Room: 214	Room: 215	Room: 219	Room: 220
	Chair: And	drea Dessen		Chair: Malla	Reddy Chilla	Chair: Ant	onia Neels				
9.00am - 9.50am	Prof Xiao	oote 13 dong Zhang ogical Macromolecules	Child Care	Keyno Prof Panč Commission for St	e Naumov	Dr Winnie	ote 15 e Wong-Ng Powder Diffraction	Software Fayre			
9.50am - 10.20am				1		Morning Tea					
	Room: 203	Room: 204	Room: 205	Room: 210	Room: 211	Room: 212	Room: 213	Room: 214	Room: 215	Room: 219	Room: 220
	Chair: Sau	lius Grazulis		Chair: Paulir	na Dominiak	Chair: Kamil	Filip Dziubek				
10.20am - 11.10am	Mr An	ote 16 dy Gotz ee on Data	Child Care	Keyno Dr Simon ( Commission on Quar	Grabowsky	Dr Ricardo Do	ote 18 nizeth dos Reis n High Pressure	Software Fayre			
11.10am - 12.10pm											
12.10pm - 1.10pm	Lunch			XRD will change over free lunch Sponsored by Bruker 12.20pm - 1.05pm		Lunch		Meeting of the Commission on Structural Chemistry 12.00pm - 1.00pm	Closed meeting of the Commission for Mathematical Crystallography 12:00pm - 12:30pm  Open meeting of the Commission for Mathematical Crystallography 12:30pm - 1.00pm	Lu	nch
	Room: 203	Room: 204	Room: 205	Room: 210	Room: 211	Room: 212	Room: 213	Room: 214	Room: 215	Room: 219	Room: 220
	Chairs: Pingwei Li	Chairs: Charles Ballard		Chairs: Hidehiro Uekusa	Chairs: Koji Yonekura & Tamir Gonen	Chairs: Andrew Goodwin	Chairs: Ricardo Donizeth dos Reis			Chairs: Françoise Damay & Ovidiu Garlea	Chairs: Nicholas Schwarz Andrew Gotz
	Session: A019 Structural Immunology	Session: A025 Diffraction Science in Virtual/Remote Settings – Remote Access to Instrumentations		Session: A102 Landscapes, Hills and Valleys: A World of Crystal Forms	Session: A039  New Approaches to the  Crystal Structure of  Pharmaceutics and  Macromolecules	Session: A075 Total Scattering Studies of Disordered Materials	Session: A046 Diffraction Studies in Dynamic Compression Experiments			Session: A053 Magnetic Symmetry and its Applications	Session: A109 Data-Driven Science: Curro Status and Outlook
	#411 - Dr Wael Awad Contributed talk 1	#1164 - Dr Ralf Flaig Contributed talk 1	Ralf Flaig	#511 - Dr Doris Braun Contributed talk 1	#1854 - Dr Michael Martynowycz Contributed talk 1	<b>#786 - Mr Thomas Nicholas</b> Contributed talk 1	#1459 - Dr Earl O'Bannon Contributed talk 1			#606 - Dr Vladimir Pomjakushin Contributed talk 1	#94 - Dr Filip Leonarsk Contributed talk 1
1.10pm - 3.30pm	#1239 - Dr Priyanka Chaurasia Contributed talk 2	#1556 - Dr Eleanor Campbell Contributed talk 2	Child Care	#1257 - A/Prof Suguru Ito Contributed talk 2	#1190 - Ms Laura Pacoste Contributed talk 2	#328 - Dr Yuanpeng Zhang Contributed talk 2	#1387 - Dr Karen Appel Contributed talk 2	Software Fayre		#232 - Prof Javier Campo Contributed talk 2	#534 - Dr Yasumasa Jo Contributed talk 2
	Jamie Rossjohn Invited Speaker 1	Dr Alun Ashton Invited Speaker 1		Prof Delia A. Haynes Invited Speaker 1	<b>Dr Max Clabbers</b> Invited Speaker 1	Prof Nan Zhang Invited Speaker 1	Dr Geun Woo Lee Invited Speaker 1			Prof Branton Campbell Invited Speaker 1	<b>Dr Max Nanao</b> Invited Speaker 1

	#1561 - Dr Jiansheng Jiang Contributed talk 3	#1489 - Dr Thomas Proffen Contributed talk 3		#1147 - Prof Kraig Wheeler Contributed talk 3	#1757 - Dr Paul Benjamin Klar Contributed talk 3	#1673 - Mr Daniele Bonavia Contributed talk 3	#52 - Dr Lisa Luhongwang Liu Contributed talk 3			#681 - Prof J. Manuel Perez Mato Contributed talk 3	#1385 - Dr Masaki Yamamoto Contributed talk 3
	#1328 - Prof Junyu Xiao Contributed talk 4	#762 - Dr Michel Fodje Contributed talk 4		#209 - Mr Jake Weatherston Contributed talk 4	#971 - Miss Yan Li Contributed talk 4	#1205 - Ms Yevheniia Kholina Contributed talk 4	Contributed talk 4			#1158 - Dr. Anna Mandziak Contributed talk 4	#1651 - Dr Stefan Brandstetter Contributed talk 4
	Prof. Toshiyuki Shimizu Invited Speaker 2	Dr Ritimukta (Rita) Sarangi Invited Speaker 2		Prof Krešo Bučar Invited Speaker 2	Saori Maki-Yonekura Cancelled Invited Speaker 2	Dr Frederick Marlton Invited Speaker 2	Dr Amy Coleman Invited Speaker 2			<b>Dr Atsushi Togo</b> Invited Speaker 2	Prof Ian Foster Invited Speaker 2
3.30pm - 4.00pm						Afternoon Tea					
	Room: 203	Room: 204	Room: 205	Room: 210	Room: 211	Room: 212	Room: 213	Room: 214	Room: 215	Room: 219	Room: 220
	Chairs: Dritan Siliqi	Chairs: Gemma de la Flor & Leopoldo Suescun		Chairs: Katharina Edkins & Doris Braun	Chairs: Jian-Min Zuo & Amelia Liu	Chairs: Maura Malinska & Simon Grabowsky	Chairs: Livia Salvati Manni			Chairs: J. Manuel Perez- Mato	Chairs: Federico Boscherini & Xiaoyi Zhang
	Session: A012 Integrative Methods Applied to Structural Biology in memoriam of Prof Raimond Ravelli	Session: A067 Crystallographic Symmetry and its Application in Material Science	Child Care	Session: A094 Crystal Engineering Applications to Pharmaceuticals	Session: A032 Mapping atomic scale structure using electron diffraction and imaging	Session: A081 Advances in Quantum Crystallography	Session: A088 Lipid Self-assembly and the Design of Lipidic Materials			Session: A060 In memoriam of Igor Dzyaloshinskii and Sergey V. Maleyev: Antisymmetric Exchange, Magnetic Chirality, from Helimagnets to Topological Spin Textures	Session: A116  Dynamical processes and transient structures underlying energy conversion: x-ray spectroscopies from fs to µs
	#1221 - Prof Charlie Bond Contributed talk 1	#11 - Prof Peter Moeck  Cancelled  Contributed talk 1		#349 - Miss Yichun Shen Contributed talk 1	#113 - Dr Daisuke Morikawa Contributed talk 1	#337 - Mr Paul Niklas Ruth Contributed talk 1	#1345 - Dr Joshua Marlow Contributed talk 1			#124 - Dr Feng Ye Contributed talk 1	#880 - Dr Bi-Hsuan Lin Contributed talk 1
4.00pm - 6.30pm	#392 - Daniella Trivella Contributed talk 2	#630 - Ms Subhashree Satapathy Contributed talk 2		#153 - Dr Rajni Miglani Bhardwaj Contributed talk 2	<b>#728 - Dr Bryan Esser</b> Contributed talk 2	#666 - Dr Helena Butkiewicz Contributed talk 2	#1105 - Dr Samuel Watts Contributed talk 2			#1623 - Werner Schweika Contributed talk 2	#1893 - Zhedong Zhang Contributed talk 2
	Prof Antonia Neels Invited Speaker 1	Prof Max Avdeev Invited Speaker 1		A/Prof Hidehiro Uekusa Invited Speaker 1	<b>Dr Colin Ophus</b> Invited Speaker 1	Prof Peter M. Weber Invited Speaker 1	Dr Liliana de Campo Invited Speaker 1	Software Fayre		Prof Junichiro Kishine Invited Speaker 1	<b>Dr Chris Milne</b> Invited Speaker 1
	#367 - Prof Bostjan Kobe Contributed talk 3	#1466 - Mr Bryce Eggers Contributed talk 3		#1373 - Mr Bhaskar Tiwari Contributed talk 3	#1809 - A/Prof Shery Chang Contributed talk 3	#1180 - Mr Michael Patzer Contributed talk 3	#340 - Dr Andrew Clulow Contributed talk 3			#317 - Dr Dmitry Khalyavin Contributed talk 3	#163 - Mr Kiyohiro Adachi Contributed talk 3
	#1498 - A/Prof Isabelle Rouiller Contributed talk 4	#1668 - Dr Dillip Pradhan Contributed talk 4		Contributed talk 4	<b>#749 - Prof Randi Holmestad</b> Contributed talk 4	#1245 - Dr Magdalena Woinska Contributed talk 4	#1545 - Dr Khay Fong Contributed talk 4			#142 - Wu Xie Contributed talk 4	Contributed talk 4
	Prof Abel Moreno Invited Speaker 2	Prof Ivanka Milosevic Invited Speaker 2		<b>Dr Amy Sarjeant</b> Invited Speaker 2	<b>Dr Ye Zhu</b> Invited Speaker 2	Dr Julia Contreras-García Invited Speaker 2	#539 - Ms Svenja Carolin Hövelmann Contributed talk 5			Dr Vladimir Pomjakushin Invited Speaker 2	Prof Lin Chen Invited Speaker 2
6.30pm - 7.00pm					<b>Dr Mariana Klementova</b> Invited Speaker 3		#1199 - Dr Orion Shih Contributed talk 6				
6.30pm - 7.00pm					•	Break	_				
7.00pm - 8.00pm						Prof Hideo Hosono Plenary Speaker					

#### Saturday 26 August

	T											
8.30am - 7.00pm						Registrat	ion Open					
	Room: 203/4	Room: 205	Room: 207	Room: 208	Room: 209	Room: 210/11	Room: 212/13	Room: 214	Room: 216	Room: 217	Room: 219	Room: 220
	Chair: Wladek Minor					Chair: Delia Haynes	Chair: John Daniels					
9.00am - 9.50am	Keynote 19 Prof Stephen K. Burley Commission on Biological Macromolecules	Child Care				Keynote 20 Prof Consiglia Tedesco Commission for Structural Chemistry	Keynote 21 Prof Shanti Deemyad Commission on High Pressure	Software Fayre				
9.50am - 10.20am						Morni	ng Tea					
	Room: 203/4	Room: 205	Room: 207	Room: 208	Room: 209	Room: 210/11	Room: 212/13	Room: 214	Room: 216	Room: 217	Room: 219	Room: 220
	Chair: Vanessa Peterson						Chair: Wei Ren					
10.20am - 11.10am	Keynote 22 Dr Clarina R Dela Cruz Commission on Neutron Scattering	Child Care					Keynote 24 Prof Mois Aroyo Commission on Mathematical and Theoretical Crystallography	Software Fayre				
11.10am - 12.10pm				Pos	sters				Closed meeting of the Commission on Quantum Crystallography 11.30am - 12.00pm	Meeting of the Council of the	Pos	ters
12.10pm - 1.10pm			Lunch			Thermo Fisher Scientific Session over free lunch 12.20pm - 1.05pm	Lun	ch	Open meeting of the Commission on Quantum Crystallography 12.00pm - 1.00pm	Asian Crystallographic Association 11.30am - 1.00pm	Lui	nch
	Room: 203/4	Room: 205	Room: 207	Room: 208	Room: 209	Room: 210/11	Room: 212/13	Room: 214	Room: 216	Room: 217	Room: 219	Room: 220
	Chairs: Claudio Ciferri & Sandra Cowan-Jacob		Chairs: Rosanna Rizzi	Chairs: Changlin Zheng & Colin Ophus	Chairs: Carla Polo & Tatiana Latchevskaia	Chairs: Andrew Cairns & Jodie Bradby			Chairs: Michele Zema	Chairs: Ivanka Milosevic & Gemma de la Flor	Chairs: Hajime Ito	Chairs: Valeska Ting & Kevin Stone
	Session: A016a Structure-based Drug Design		Session: A024 New Software in Powder Diffraction	Session: A031 Advances in Electron Crystallography Methods for Solving Crystal Structures	Session: A089a Coherent scattering methods using X-rays or electrons	Session: A045 Using High-pressure Diffraction to Design and Understand Functionality			Session: A052 Year of Mineralogy	Session: A066 Subperiodic Symmetry Groups and their Applications	Session: A103 Mechanochemistry Meets Crystal Engineering	Session: A073 Transient Phenomena and in Operando Experiments and Modelling
	#179 - Mrs Tatjana Barthel Contributed talk 1		#862 - Dr Andrew Sazonov Contributed talk 1	#1426 - Dr Laura Clark Contributed talk 1	#1628 - Dr Ana Diaz Contributed talk 1	#363 - A/Prof. Vittoria Pischedda Contributed talk 1			#893 - Prof José Miguel Delgado Contributed talk 1	#1312 - Mr Rovin Santos Contributed talk 1	<b>#522 - Mr Yusaku Nakajima</b> Contributed talk 1	#714 - Dr Laura Folkers Contributed talk 1
1.10pm - 3.30pm	#1272 - Prof Tian Hua Contributed talk 2		#135 - Dr Matthew Rowles Contributed talk 2	#1604 - Dr Alke Meents Contributed talk 2	#210 - Dr Ruslan Kurta Contributed talk 2	#459 - Dr Isabelle Jones Contributed talk 2			Contributed talk 2	#111 - Dr Mark Tomenes Contributed talk 2	#654 - Dr Arnaud Grosjean Contributed talk 2	#878 - A/Prof Neeraj Sharma Contributed talk 2
•	Prof. Patrick Sexton Invited Speaker 1	Child Care	Dr Alan Coelho Invited Speaker 1	Prof Sandra Van Aert Invited Speaker 1	Dr Marie-Ingrid Richard Invited Speaker 1	Dr Zhidan Zeng Invited Speaker 1		Software Fayre	Prof Razvan Caracas Invited Speaker 1	Prof Pavel V. Avramov Invited Speaker 1	Invited Speaker 1	Prof Claire White Invited Speaker 1
	#930 - Prof Renae Ryan Contributed talk 3		#953 - Dr Saulius Gražulis Contributed talk 3	Contributed talk 3	#887 - Dr Kartik Ayyer Contributed talk 3	#1235 - Dr Banele Vatsha Contributed talk 3			Contributed talk 3	#1365 - Dr Gotzon Madariaga Contributed talk 3	#143 - Dr Szymon Sobczak Contributed talk 3	#1718 - Dr Mark Warren Contributed talk 3
	#440 - Dr Jeff Perry Contributed talk 4		Haotong Liang Invited Speaker 2	#582 - Ms Laura Samperisi Contributed talk 4	#589 - Mr Daniyal Younas Contributed talk 4	Contributed talk 4			Contributed talk 4	Contributed talk 4	#647 - Dr Avantika Hasija Contributed talk 4	#587 - Mr Bryce Mullens Contributed talk 4
	Prof Alice Vrielink Invited Speaker 2		#1977 - Dr Thomas Degen Contributed talk 4	<b>Dr Amelia Liu</b> Invited Speaker 2	Prof Rafal Dunin-Borkowski Invited Speaker 2	<b>Dr David Ashworth</b> Invited Speaker 2			Prof Giuseppe Cruciani Invited Speaker 2	Invited Speaker 2	Invited Speaker 2	Dr Ashkan Salamat Invited Speaker 2
				#1136 - A/Prof Peng Wang								

2.00pm - 3.00pm						"How I fell in love v	Lecture with Crystallography" ifer Martin					
3.30pm - 4.00pm						Aftern	oon Tea					
	Room: 203/4	Room: 205	Room: 207	Room: 208	Room: 209	Room: 210/11	Room: 212/13	Room: 214	Room: 216	Room: 217	Room: 219	Room: 220
	Chairs: Claudio Ciferri & Sandra Cowan-Jacob		Chairs: Marlena Gryl & Parthapratim Munshi	Chairs: Junliang Sun & Hongyi Xu	Chairs: Carla Polo & Tatiana Latchevskaia		Chairs: William Ratcliff & Maxim Avdeev		Chairs: Elke Scholten & Fernanda Peyronel	Chairs: Kotaro Fujii	Chairs: Chris Ritchie & Patrice Kenfack Tsobnang	Chairs: Thomas Penfold & Maria K. Chan
	Session: A016b Structure-based Drug Design		Session: A082 Materials Properties by Quantum Crystallography	Session: A038 Crystallography of Nanocrystalline Porous Materials	Session: A089b Coherent scattering methods using X-rays or electrons		Session: A074  Methods for the  Determination and Analysis of  Magnetic Structures		Session: A092 Scattering methods for Structural Elucidation in Food Systems	Session: A096 Progress and Application of Bond Valence Method	Session: A101 Organic-inorganic Hybrid Materials	Session: A115 and A117 Applications of Machine Learning to X-ray Spectroscopy and Scattering and Putting Pressure on Complementary X-ray
	#410 - Dr Stefan Hermans Contributed talk 1		#1590 - Prof Xiao-Ming Jiang Contributed talk 1	#1095 - Prof Valeska Ting Contributed talk 1	#885 - Mr Abishek Mall Contributed talk 1		#396 - Dr Lester Barnsley Contributed talk 1		#1443 - Prof Cristiano Oliveira Contributed talk 1	#1351 - Mr Kohei Matsuzaki Contributed talk 1	#1439 - Prof Tomoji Ozeki Contributed talk 1	Dr Yang Ding Invited Speaker 1 (25min)
4.00pm - 6.30pm	#1663 - Dr Sebastian Guenther Contributed talk 2	Child Care	#1175 - Mr Yaser Balmohammadi Contributed talk 2	#724 - Dr Yi Zhou Contributed talk 2	#1175 - Dr Chufeng Li Contributed talk 2		#220 - Dr Ping Miao Contributed talk 2	Software Fayre	#1753 - Dr Fernanda Peyronel Contributed talk 2	#1354 - Mr Kei Saito Contributed talk 2	#1524 - Dr Ashley Sutton Contributed talk 2	#1085 - Mr Luke Watson Contributed talk 1 (15min)
	#1218 - Dr Andrew Thompson Contributed talk 3	Child Care	Prof Eiji Nishibori Invited Speaker 1	<b>Dr A. Ken Inge</b> Invited Speaker 1	Prof Henry Chapman Invited Speaker 1		Dr Stuart Calder Invited Speaker 1	solumeragie	Prof Elliot Paul Gilbert Invited Speaker 1	Dr Sacha Fop Invited Speaker 1	Invited Speaker 1	Dr Valerie Briois Invited Speaker 2 (25min)
	#1730 Dr Roman Hillig Contributed talk 4		#750 - Ms Ashi Singh Contributed talk 3	#1394 - Ms Sofiia Butonova Contributed talk 3	#1672 - Yuriy Chuskin Contributed talk 3		#1161 - Dr Piotr Fabrykiewicz Contributed talk 3		#1432 - A/Prof Elke Scholten Contributed talk 3	Contributed talk 3	#1479 - A/Prof Aal Seham Contributed talk 3	#211 - Dr William Ratcliff Contributed talk 2 (15min)
	#1324 - Dr Benjamin Walters Contributed talk 5		#677 - Dr Natalia Alvarez Contributed talk 4	#185 - Ms Laura Samperisi Contributed talk 4	#1265 - Dr Cameron Kewish Contributed talk 4		#371 - Dr Martin Meven Contributed talk 4		#1412 - Dr Theresia Heiden- hecht Contributed talk 4	Contributed talk 4	#176 - Dawid Drozdowski Contributed talk 4	#1399 - Dr Tudur David Contributed talk 3 (25min)
	#18 - Dr Debanu Das Contributed talk 6		Prof Bo Brummerstedt Iversen Invited Speaker 2	Prof Daliang Zhang Invited Speaker 2	<b>Dr Cathal Cassidy</b> Invited Speaker 2		Prof Tsuyoshi Kimura Invited Speaker 2		<b>Dr Elena Simone</b> Invited Speaker 2	Prof Kazuhiro Mori Invited Speaker 2	Invited Speaker 2	#846 - Prof Christopher Chantler Contributed talk 4 (15min)
6.30pm - 7.00pm						Br	reak					

7.00pm - 8.00pm

Dr Junko Yano

Plenary Speaker

#### **Sunday 27 August** Day 6 **Registration Open** 9.30am - 4.00pm 9.50am - 10.20am Morning Tea Room: 203/4 Room: 205 Room: 208 Room: 209 Room: 210/11 Room: 214 Room: 216 Room: 217 Room: 219 Room: 220 Chair: Xiao Dong Chair: Marcia C A Fantini Chair: Yaroslav Khimyak 10.20am - 11.10am Keynote 27 Keynote 25 Keynote 26 Child Care Software Favre **Prof Christian Bonho** Prof Yoshiki Higuchi **Prof Ian Robinson** Commission on NMR Commission on Biological Commission on Synchrotron Crystallography and Related Macromolecules and XFEL Radiation Methods 11.10am - 12.10pm Posters Closed meeting for the **Commission on Electron** 12.10pm - 1.10pm Lunch Lunch Crystallography 12:00pm - 1:00pm Room: 203/4 Room: 205 Room: 207 Room: 209 Room: 210/11 Room: 212/13 Room: 214 Room: 216 Room: 217 Room: 219 Room: 220 Chairs: Airlie McCoy & José-Chairs: Miki Senda and Yu-Chairs: Santosh Panjikar & Chairs: P.K. Madhu & Yusuke Chairs: Valentina Dichiarante Chairs: Cora Lind-Kovacs & Chairs: Emma McCabe & Chairs: A. Sundaresan & Chairs: Joanne Etheridge & María Carazo Garcia & Luigi Chairs: Wolfgang W. Schmal Chih Lo Martin Lutz Nishiyama & Catharine Esterhuysen **Helen Brand Anthony Phillips Fabio Denis Romero Brent Nannenga** Vitagliano A009 & A010 Use and Comparison of Session: A069 Session: A043 Session: A078 Session: A057 Predicted Models from Session: A034 Structural chemistry at the Session: A100 Session: A022 Session: A048 Session: A005 Crystal Growth and interface of diffraction, The Arsenal of What Every Crystallographer Crystal and Magnetic Primary Sequence in Quantifying the Electrostatic Computing Intermolecular Functionality from Broken Characterization of Potential with Accurate nuclear magnetic resonance Supramolecular Interactions Should Know About Powder Structures of Novel Structural Biology and Deep Sample Preparation Interactions Inversion Symmetry Biominerals and Biomimetics for Crystal Engineering Diffraction Learning & Artificial Electron Diffraction Studies Perovskites and other spectroscopic and Intelligence in Structural computational tools Biology #899 - Prof Olga Frank-#1210 - Prof Fernando J. #202 - Ms Barbara Olech #1679 - Dr Gerhard Hofei #461 - Dr Anton Savchenko #1286 - A/Prof David Turner #725 - Dr Andy Fitch #554 - Ms Tina Weigel #1344 - Mr Alex Brown #1408 - Mr Xin Zhang Kamenetskaya Lahoz Contributed talk 1 1.10pm - 3.30pm Child Care #844 - Prof Catharine #1107 - Dr Dubravka Sisak **Software Fayre** #1585 - Dr Roxanne P. Smith #662 - Miss Jana Storsberg #1080 - Dr David Bryce #1519 - A/Prof Marlena Gryl #1743 - Prof Shinobu Aoyagi 230 - Prof Yuichi Shimakaw #122 - Dr Dennis Piehl #526 - Prof Kenji Tsuda Esterhuyser Contributed talk 2 Prof. Takeshi Murata Dr Peter Spackman Stefano Checchia Prof Giuseppe Resnati Dr Matthew Rowles A/Prof Kenta Kimura **Prof Patrick Woodward** Prof Daisuke Kihara A/Prof Philip Nakashima Invited Speaker 1 #501 - Dr Adrian Rodriguez-#1673 - Dr Angshuman #476 - Prof Joachim #690 - Dr. Yusuke Yamada #801 - Dr Christian Jelsch #1223 - Dr Munehiro Inukai #1811 - Mr Adam Corrao #1855 - Tristian Bepler #1340 - Dr Emre Yörük #794 - Dr Rvan Morrow Breternitz Contributed talk 3 #1264 - Mrs Martyna Mateia #1788 - A/Prof Kyeong Kyu #665 - Mr Daniyal Younas #304 - Dr Maura Malinska #792 - Harry James Lloyd #1550 - Wayne Hendrickson #1615 - Dr Scott Findlay Contributed talk 4 Dr Mitchell Miller Prof Henrik Birkedal Dr Giulia Mollica A/Prof Louise Dawe Dr Helen Maynard-Casely Prof J. Paul Attfield Prof Jose Maria Carazo Dr Lukáš Palatinus Invited Speaker 2 3.30pm - 4.00pm Afternoon Tea Room: 210/11 Room: 203/4 Room: 205 Room: 207 Room: 208 Room: 209 Room: 212/13 Room: 214 Room: 216 Room: 217 Room: 219 Room: 220 Chairs: Dorothee Liebschner Chairs: Doris Braun & Chairs: Ana Diaz & Cameron Chairs: Nicolas Claiser & Chairs: Kang Min Ok & Chairs: Josie Auckett & Jette Chairs: Grace Causer & Chairs: Benoit Guillot Chairs: Panče Naumov & Oleg Sobolev **Andrew Wildes Sharmarke Mohamed** M. Kewish Yoshiharu Sakurai Chandrasekar Rajadurai Oddershede Session: A070 Session: A029 Polymorphism, Functional Session: A099 Session: A108 Session: A083 Grain Boundary and Session: A011 Session: A071 Session: A085 Session: A064 Materials and Structural Optically and Electronically X-ray Ptychography: Recent Quantum Crystallography Intergranular Phenomena Validation of Biological Polarised Neutrons - Future Quantum Approaches in New Opto-electronic Transformations: Active Materials Developments and hallenges and Opportunities Investigated by Diffraction-Macromolecular Structure Directions Biocrystallography Functional Materials Inderstanding Properties and **Applications** for Magnetic Materials based Microstructural Disorder Imaging Methods #1429 - Dr Xiaoxu Guo #833 - Mr Michal Gucwa #1641 - Dr Jian-rui Soh #1232 - A/Prof Birger Dittrich #1994 - Mr Ahmadi Permana #484 - Dr Christopher Garvey #106 - Ian Robinson #1802 - Miss Sabrina Grenda #1121 - Mrs Huanyu He Contributed talk 1 Contributed talk 1

4.00pm - 6.30pm	#1295 - Dr Laura Ciacchi Contributed talk 2	Child Care	#1857 - Dr David Cortie Contributed talk 2	#167 - Dr Marta Kulik Contributed talk 2	#1182 - Dr Krishnayan Basuroy Contributed talk 2	#1203 - Miss Astghik Danghyan Contributed talk 2	#182 - Dr Maik Kahnt Contributed talk 2	Software Fayre	#1472 - Dr Jey-Jau Lee Contributed talk 2	#181 - Dr Galina Gurieva Contributed talk 2	#657 - Dr Erik Lauridsen Contributed talk 2	
	<b>Dr Ikuko Miyaguchi</b> Invited Speaker 1		Dr Francoise Damay Invited Speaker 1	Prof Ulf Ryde Invited Speaker 1	A/Prof Brijith Thomas Invited Speaker 1	Prof Chandrasekar Rajadurai Invited Speaker 1	<b>Dina Carbone</b> Invited Speaker 1		Hiroshi Sakurai Invited Speaker 1	Prof Ling Chen Invited Speaker 1	Prof Darren Pagan Invited Speaker 1	
	#1277 - Dr Luigi Vitagliano Contributed talk 3		#1614 - Dr Werner Schweika Contributed talk 3	#151 - Dr Lorraine Andrade Malaspina Contributed talk 3	#74 - Dr Hema Kuntrapakam Contributed talk 3	#1694 - Miss Manjiri Choudhari Contributed talk 3	#283 - Thomas Aidukas Contributed talk 3		#948 - Ms Nilofar Kurawle Contributed talk 3	#1019 - Dr Julia Payne Contributed talk 3	#1671 - Mr Aditya Shukla Contributed talk 3	
	#1448 - Miss Abbey Butler Contributed talk 4		#1250 - A/Prof Benjamin Frandsen Contributed talk 4	#1702 - Prof Maciej Kubicki Contributed talk 4	#1770 - Prof Yaroslav Khimyak Contributed talk 4	Contributed talk 4	#333 - Mr Francisco Mateus Cirilo da Silva Contributed talk 4		#1478 - Dr Feng Ye Contributed talk 4	#1097 - Dr Asma Hasil Contributed talk 4	#843 - Dr Hrishikesh Bale Contributed talk 4	
	Dr Christopher Williams Invited Speaker 2		Vasile Ovidiu Garlea Invited Speaker 2	Dr Julia Contreiras Garcia Invited Speaker 2	A/Prof Mingoo Jin Invited Speaker 2	Prof Jack Clegg Invited Speaker 2	Xiaojing Huang Invited Speaker 2		Prof Dominique Luneau Invited Speaker 2	#814 - Dr Durga Prasad Karothu Invited Speaker 2	Dr Jaemyung Kim Invited Speaker 2	
		<u> </u>		·		·	·		·	<u> </u>		Room: 219/220
7.30pm - 10.30pm												General Assembly 3 7.30pm - 10.30pm

#### **Monday 28 August** Day 7 8.30am - 6.00pm **Registration Open** Room: 203/4 Room: 205 Room: 209 Room: 210/11 Room: 212/13 Room: 214 Room: 216 Room: 219 Room: 220 Room: 207 Room: 208 Room: 217 Chairs: Radomir Kuzel & Susan Chair: Michael Glazer Chair: Annalisa Guerri 9.00am - 9.50am A. Bourne **Child Care** Kevnote 31 Software Fayre Bragg Prize Dr Airlie McCoy Struchkov Prize **Prof Arkadiy Simonov** Dr Robert Fayzullin nmission for Biological Macromolcules 9.50am - 10.20am **Morning Tea** Room: 203/4 Room: 205 Room: 207 Room: 208 Room: 209 Room: 210/11 Room: 212/13 Room: 214 Room: 216 Room: 217 Room: 220 Chair: Angus Wilkinson Chair: Ozeki Tomoji 10.20am - 11.10am **Gjonnes Medal** Kevnote 32 Keynote 33 Child Care Software Fayre Prof Jian-Min Zuo Prof Ram Seshadri Prof Hoi Ri Moon Commission for Structural Commission for Powder Diffraction Chemistry 11.10am - 12.10pm **Posters** 12.10pm - 1.10pm Lunch Room: 205 Room: 212/13 Room: 217 Room: 203/4 Room: 207 Room: 208 Room: 209 Room: 210/11 Room: 216 Room: 219 Room: 220 Chairs: Hiroshi Sekiguchi & Chairs: Jan Rohlicek & Ma Chairs: Ichiro Hisaki & Sareeya Chairs: Carlotta Giacobbe & Chairs: María Cristina Nonato, Shao-Chairs: Dominik Oberthür and Chairs: Richard Mole & Annie Chairs: Edmund Welter & **Chairs: Prof Siegbert Schmid** Chairs: Sébastien Merkel Charlie Bond Louise Antonette De Las Penas Amelie Rochet Liang Zheng & Alison Edwards Bureekaew Alessandra Henkel Powell Session: A026 and A106 Session: A030 Session: A110 Session: A114 Session: A023 Session: A058 Crystallographic Education – Building Session: A008 Session: A107 Session: A051 Multigrain Crystallography Room-temperature Serial New Opportunities in X-ray **Comparing Crystal Structures** New Phenomena and Community in the 21st Century and Biomolecules for a Sustainable Chairs: Giuliana Aquilanti Multicrystal Indexings, and Design and application of Snapshot Micro-Applied Mineralogy and Spectroscopy at Ultra Low and Data Applications in Molecular Crystallography for the Next Future Microstructures in High porous materials rystallography: Highlights from Sustainability mittance Synchrotron Sources Generation: Innovation, Equity, Magnets Pressure Experiments XFELs and Synchrotrons Diversity and Inclusion #1189 - Ms Sofie Stampe #1216 - Dr Mihwa Lee #572 - Prof Jens R. Stellhorn #688 - Mr Matt Bright #1292 - Sébastien Merkel #977 - Prof Christopher Sumby #221 - Miss Kara Zielinski #1617 - Ms Theresa Lender #394 - Prof Kiyotaka Asakura #19 - Prof John Helliwell Leiszner Contributed talk 1 #950 - Mr Loïc Bénariac-#1700 - Nydia Roxana Varela-1.10pm - 3.30pm #1744 - Dr Jeremy Karl #1386 - Dr Olivier Berteau #669 - Dr Natalie Johnson #166 - Dr Amanpreet Kaur #937 - A/Prof Sabine Botha #744 - Prof Javier Campo #324 - Dr Paul D. Quinn #261 - Dr Nico Graw Child Care Software Fayre Cockcroft Rosales Doumal Contributed talk 2 Contributed talk 1 Contributed talk 2 **Prof Chien-Lung Wang** Dr Tsunetomo Yamada Prof Vitaliy Kurlin Li Zhang Prof Karena Chapman Dr Ian Kern A/Prof. Serena C. Tarantino Ms Hannah Hedegaard Nielse Prof Yukio Takahashi Dr Joseph Ferrara Invited Speaker 1 #1475 - Dr Dorothee #342 - Dr Manuel Guizar #173 - Mr Cristiano Mota Dr. Priva Subramanian #1462 - Dr Shuhua Yuan #199 - Prof Angiolina Comotti #1520 - Dr Andrew Martin #1713 - Dr Rvo Yamane #589 - Mr Miguel Pardo #362 - Dr Sebastián Klinke Liebschner Sicairos Contributed talk 3 Invited Speaker 2 Contributed talk 3 #148 - Prof Santiago Garcia-#1771 - Prof Michele Zema #1127 - Zhu Qiao #2951 - Mr Daniel Widdowso #637 - Dr Thomas Fellowes #1425 - Ms Anaïs Chretien #1521 - Richard Mole #540 - Dr Majid Kazemian Contributed talk 4 Contributed talk 4 Granda Contributed talk 4 Dr Taiyo Yoshioka **Prof. Tomonari Dotera Prof Paulo Salbego** Claire Zurkowski **Andreas Schneemann** Dr Swagatha Ghosh Dr Andrew Allen Yuko Hosokoshi Hirosuke Matsui #939 - A/Prof Leopoldo Suescun Invited Speaker 2 Invited Speaker 3 Invited Speaker 2 Contributed talk 5 #730 - Dr Natalia Alvarez Contributed talk 6 3:30pm - 4:00pm #2135 - Miss Katrina Wruck

Afternoon Tea

3.30pm - 4.00pm

Contributed talk 7

	Room: 203/4	Room: 205	Room: 207	Room: 208	Room: 209	Room: 210/11	Room: 212/13	Room: 214	Room: 216	Room: 217	Room: 219	Room: 220
	Chairs: Gaya Amarasinghe & Alice Vrielink		Chairs: Fabrizia Foglia & William Brant	Chairs: Manabu Hoshino	Chairs: Rebecca Scatena & Sajesh P. Thomas	Chairs: Wei-Tsung Chuang	Chairs: John Helliwell			Chairs: Luis Elcoro & Anna Sokolova	Chairs: Giuliana Aquilanti & Aline Ribeiro Passos	Chairs: Hanna Dabkowska & Santiago Garcia-Granda
	Session: A015 Structures of Very Large Assemblies		Session: A072 Understanding Energy System Processes and Function	Session: A079 Dealing with the Data Deluge	Session: A044 High-pressure Quantum Crystallography	Session: A087 Simultaneous Small-angle Scattering of Soft Materials During Deformation: Recent Developments in rheoSAS and in Operando Deformation	Session: A119 Interoperability of Crystallographic Data and Databases			Session: A061 Magnetism in Topological Materials	Session: A113 Materials for Advanced Energy Technologies	Session: A120 IUCr 75th Anniversary
	#1515 - Prof Ning Gao Contributed talk 4	Child Care	#1323 - Dr Indri Adilina Contributed talk 1	#70 - Dr Rosanna Rizzi Contributed talk 1	#55 - Prof Arthur Haozhe Liu Contributed talk 1	#1338 - Ms Vo Ngan Contributed talk 1	#311 - Mx Thomas Smith Contributed talk 1			#1667 - Dr Jian-Rui Soh Contributed talk 1	#1477 - Dr Angelo Mullaliu Contributed talk 1	Featuring presentations from: Prof Brian McMahon Prof Edward (Ted) Baker
4.00pm - 6.30pm	#1493 - Dr Pierre Legrand Contributed talk 2		#547 - Miss Ida Nielsen Contributed talk 2	#622 - Dr Takafumi Hawai Contributed talk 2	#66 - Prof Krzysztof Wozniak Contributed talk 2	#127 - Prof Sanjeeva Murthy Contributed talk 2	#1377 - Dr Toby Blundell Contributed talk 2	Software Fayre		#494 - Dr Grace Causer Contributed talk 2	#1289 - Dr Sofia Diaz-moreno Contributed talk 2	Prof Sven Lidin Prof Malcolm Cooper Mr Peter Strickland
	Prof Brett Collins Invited Speaker 1		Dr Anatoliy Senyshyn Invited Speaker 1	Prof Kanta Ono Invited Speaker 1	Prof Anna Makal Invited Speaker 1	Prof Michelle Calabrese Invited Speaker 1	Prof Daumantas Matulis Invited Speaker 1			A/Prof Catherine Pappas Invited Speaker 1	Dr Mali Balasubramanian Invited Speaker 1	Prof Michele Zema Prof Delia Haynes Dr Helen Maynard-Casely Dr Annalisa Guerri
	#387 - Dr Emily Furlong Contributed talk 3		#503 - Mr Keenan Smith Contributed talk 3	#879 - Dr Zdenek Matej Contributed talk 3	#449 - Mr Hayden Robinson Contributed talk 3	#190 - Dr Andreas Keilbach Contributed talk 3	#1535 - Soorya Kabekkodu Contributed talk 3			#239 - Prof Javier Campo Contributed talk 3	#1505 - Dr Valérie Briois Contributed talk 3	A/Prof Louise Dawe A/Prof Leopoldo Seuscun Prof Yuki Kimura
	#1509 - Ms Evie Mansfield Contributed talk 1		Contributed talk 4	#346 - Dr Monty Cosby Contributed talk 4	Contributed talk 4	#1341 - Dr Jung-Ren Huang Contributed talk 4	#2009 - Mr Brian McMahon Contributed talk 4			#1122 - Mr George Wood Contributed talk 4	#1258 - Dr Abhijeet Gaur Contributed talk 4	Prof Gautamn Desiraju Prof Mike Glazer Prof Yuji Ohashi Prof Sine Larsen
	Sheemei Lok Invited Speaker 2		Invited Speaker 2	<b>Dr Jana Thayer</b> Invited Speaker 2	Prof Ranga Dias Invited Speaker 2	Prof Roland Kádár Invited Speaker 2	Miss Suzanna Ward Invited Speaker 2			<b>Zhida Song</b> Invited Speaker 2	Prof Stanislav Fedotov Invited Speaker 2	Prof Marvin Hackert Dr Alex Ashcroft Prof Luc Van Meervelt
6.30pm - 7.30pm			1	'	'		before party vay to Melbourne Museum				'	'
7.30pm - 11.30pm					II	· ·	seum' Congress Celebration	Party				

Tuesday 29 August  Day 8																
8.30am - 4.00pm								Registration Open								
9.00am - 10.00am	Prof Mark Spackman Plenary Speaker															
10.00am - 10.20am								Morning Tea								
10.20am - 11.10am	Room: 203	Room: 204	Room: 205	Room: 207	Room: 208	Room: 209	Room: 210	Room: 211	Room: 212	Room: 213	Room: 214	Room: 216	Room: 217	Room: 219	Room: 220	
	Chair: Santosh Panijkar						Chair: Paula Dominiak									
	Dr Kare	Keynote 34 Dr Karen Davies Commission on Biological Macromolecules					Prof T.N.	note 35 . Guru Row antum Crystallography			Software Fayre					
11.10am - 12.10pm		Posters														
12.10pm - 1.30pm		Lunch														
1.30pm - 3.50pm	Room: 203	Room: 204	Room: 205	Room: 207	Room: 208	Room: 209	Room: 210	Room: 211	Room: 212	Room: 213	Room: 214	Room: 216	Room: 217	Room: 219	Room: 220	
	Chairs: Andrzej Joachimiak	Chairs: Ella Schmidt	Child Care	Chairs: Brinda Vallat & John Helliwell		Chairs: Marjorie Senechal & Vitaliy Kurlin	Chairs: Tuan Va	Chairs: Dmitry Khalyavin & Clarina Dela Cruz	Chairs: Yumi Yakiyama & Kana M. Sureshan	Chairs: David Turner	Software Fayre			Chairs: Andrew Whitten		
	Session: A018 Viruses	Session: A003 Composite and Incommensurate Modulated Crystals: Structural and Physical Properties		Session: A014 Databases and Data Management		Session: A065 Different Approaches to Comparing Crystal Structures in Massive Datasets	Session: A047 Crystallography in Space Research	Session: A054 Methods for the Determination and Analysis of Magnetic Structures for Powders and Single Crystals	Stimuli-responsive Crystals	Session: A095  Dynamic Aspects of Crystals				Session: A086 SANS for Biomolecular Function and Cellular Organization		
	#1485 - Dr Dmitrii Zabelskii Contributed talk 1	#292 - Prof Thomas Doert Contributed talk 1		#785 - Ms Kathryn Janzen Contributed talk 1		#1868 - Jan Rohlicek Contributed talk 1	#1134 - Dr David Blake Contributed talk 1	#329 - Dr Claudia Mondelli Contributed talk 1	#112 - Ms Mami Isobe Contributed talk 1	Contributed talk 1				#1706 - Dr Anthony Duff Contributed talk 1		
	#1705 - Dr Naveen Vankadari Contributed talk 2	#823 - Dr Marc De Biossieu Contributed talk 2		#790 - Ms Christine Zardecki Contributed talk 2		#667 - Dr Nicholas Francia Contributed talk 2	#398 - Mr Nicholas Stapleton Contributed talk 2	#851 - Dr Uthayakumar Sivaperumal Contributed talk 2	#1513 - Dr Hunter Windsor Contributed talk 2	r #474 - Mr Shamim Ahmad Contributed talk 2				#1343 - Dr Alexander Grishaev Contributed talk 2		
	Dr Gaya Amarasinghe Invited Speaker 1	<b>Dr Igor Levin</b> Invited Speaker 1		<b>Dr Suzanna Ward</b> Invited Speaker 1		Mr Daniel Widdowson Invited Speaker 1	#1159 - Prof Yuki Kimura Invited Speaker 1	A/Prof Roger D. Johnson Invited Speaker 1	Prof Hajime Ito Invited Speaker 1	Prof Sharmarke Mohamed Invited Speaker 1				Eric Bryant Gibbs Invited Speaker 1		
	#1153 - Prof Chun-Jung Chen Contributed talk 3	#276 - Prof Shunta Harada Contributed talk 3		#1494 - Prof Piotr Sliz Contributed talk 3		#171 - Dr Gemma De La Flor Martin Contributed talk 3	#109 - Dr Helen E. A. Brand Contributed talk 3	Contributed talk 3	#694 - Mr Amit Mondal Contributed talk 3	#676 - Mr Johnathan Bulled Contributed talk 3				Contributed talk 3		
	Contributed talk 4	#567 - Dr Petr Veřtát Contributed talk 4		Prof Genji Kurisu Invited Speaker 2		#231 - Prof Ma Louise Antonette De Las Peñas Contributed talk 4	#828 - Dr Michael Jones Contributed talk 4	Contributed talk 4	#305 - Prof Kristof Van Hecke Contributed talk 4	#575 - Mr Shodai Hasebe Contributed talk 4				Contributed talk 4		
	Ms Ruijie Yu Invited Speaker 2	Dr Berthold Stoeger Invited Speaker 2				Mr Matt Bright Invited Speaker 2	Invited Speaker 2	Dr Rebecca L. Dally Invited Speaker 2	Dr. Ejaz Ahmed Invited Speaker 2	Mr Johnathan Bulled Invited Speaker 2				<b>Dr Marie Lycksell</b> Invited Speaker 2		
3.50pm - 4.30pm						_	1	Afternoon Tea		1				-		
4.30pm - 5.30pm							61	osing ceremony and awa	d.							