

Conference Agenda

Session Overview

Date: Wednesday, 11/Aug/2021

<p>9:00am - 6:30pm</p> <p>virtual</p>	<p>School - Electron: Electron Crystallography School Session Chair: Xiaodong Zou Session Chair: Louisa Meshi Session Chair: Lukáš Palatinus Website - virtual</p>
<p>9:00am - 6:30pm</p> <p>virtual</p>	<p>Workshop - Data: When should small molecule crystallographers publish raw diffraction data? Session Chair: Amy Sarjeant Session Chair: Simon John Coles Website - virtual</p>

Date: Thursday, 12/Aug/2021

8:30am - 4:30pm Holiday Inn	School - Aperiodic: Workshop on Aperiodic and Magnetic Structure for Beginners Session Chair: Václav Petříček Session Chair: Margarida Henriques Website
9:00am - 4:00pm virtual	Workshop CCDC/FIZ: CSD and ICSD workshop Session Chair: Suzanna Ward Session Chair: Annett Steudel Website
9:00am - 6:30pm virtual	School - Electron 2: Electron Crystallography School Session Chair: Xiaodong Zou Session Chair: Louisa Meshi Session Chair: Lukáš Palatinus Website
9:00am - 6:30pm virtual	Workshop - Data2: When should small molecule crystallographers publish raw diffraction data? Session Chair: Amy Sarjeant Session Chair: Simon John Coles Website

Date: Friday, 13/Aug/2021

8:30am - 4:30pm Holiday Inn	School - Aperiodic 2: Workshop on Aperiodic and Magnetic Structure for Beginners Session Chair: Václav Petříček Session Chair: Margarida Henriques Website
8:30am - 4:30pm virtual	Workshop - Olex: Olex2 workshop Session Chair: Horst Puschmann Website
9:00am - 5:00pm virtual	School - Electron 3: Electron Crystallography School Session Chair: Xiaodong Zou Session Chair: Louisa Meshi Session Chair: Lukáš Palatinus Website
9:00am - 5:00pm virtual	Workshop - ICDD: ICDD workshop Session Chair: Thomas Nelson Blanton Session Chair: Jose Miguel Delgado Virtual workshop

Date: Saturday, 14/Aug/2021

9:00am - 3:00pm PCC	Workshop - MX: MX Raw image data and metadata, formats and validation Website
9:00am - 4:30pm PCC	Workshop - WDQA: Data quality assesment Website
5:00pm - 5:50pm	Opening: Opening ceremony
5:50pm - 6:50pm	Opening music: Music
7:10pm - 8:00pm	Ewald: Ewald prize lecture Olga Kennard
8:00pm - 10:00pm Exhibition and poster area	Welcome: Welcome drink and refreshment

Date: Sunday, 15/Aug/2021

9:00am - 9:50am	KN-1: The symbiosis of cryo-EM and X-ray crystallography in structure determination of large macromolecular systems Session Chair: Marcin Nowotny Holger Stark
9:00am - 9:50am	KN-2: Quantum Crystallography: Past, Present, and Future Session Chair: Krzysztof Wozniak Dylan Jayatilaka
9:00am - 9:50am	KN-3
9:50am - 10:20am Exhibition and poster area	Morning break 1: Exhibition, posters, coffee/tea
10:20am - 12:45pm	MS-1: Structural bioinformatics Session Chair: Janusz Marek Bujnicki Session Chair: Jiri Cerny Invited: Zhichao Miao (UK)
10:20am - 12:45pm	MS-2: Validation of cryoEM structures and maps Session Chair: Jose-Maria Carazo Session Chair: Elena Orlova Invited: Florence Tama (Japan), Pavel Afonine (USA), G. Kleywegt (Germany)
10:20am - 12:45pm	MS-3: Crystallographic approaches for designing new framework materials (including post-synthetic modification) Session Chair: Yue-Biao Zhang Session Chair: Sergei Alexandrovich Sapchenko
10:20am - 12:45pm	MS-4: Quantum crystallography challenges and newest accomplishments Session Chair: PIERO MACCHI Session Chair: Dietmar Stalke Invited: Alessandro Genoni (France), Nicolas Claiser (France)
10:20am - 12:45pm	MS-5a: Crystal structure prediction Session Chair: Qiang Zhu Session Chair: Rajeev Ahuja Invited: Ivan Kruglov (Russia), Graeme Day (UK)
10:20am - 12:45pm	MS-6: Application of electron crystallography to functional materials Session Chair: Holger Klein Session Chair: Karla Balzuweit Invited: Mauro Gemmi (Italy), Maria Roslova (Germany)
10:20am - 12:45pm	MS-7: High throughput vs. careful planning: How to get the best data? Session Chair: John Richard Helliwell Session Chair: Selina Lea Sophie Storm Invited: Danny Axford (UK), Petrus Zwart (USA)
10:20am - 12:45pm	MS-8: Social media and new frontiers for spreading crystallographic Session Chair: Andrea Ienco Session Chair: Helen Maynard-Casely Invited: Delphine Chenevier (France), Rhiannon Morris (Australia)
10:20am - 12:45pm	SF-1: Software Fayre 1 Session Chair: Martin Lutz http://www.cryst.chem.uu.nl/lutz/
12:45pm - 2:45pm	ECA-0: ECA EC meeting ECA EC meeting
12:45pm - 2:45pm Exhibition and poster area	Lunch 1: Exhibition, posters, lunches
1:15pm - 2:45pm	CS-1: Commercial session 20 min company presentations
2:45pm - 3:45pm	MS-5b: Crystal structure prediction Session Chair: Qiang Zhu Session Chair: Rajeev Ahuja
2:45pm - 5:10pm	MS-09: Structure guided drug design and antibiotic resistance targets Session Chair: Begoña Heras Session Chair: Anton V. Zavalov Invited: Vibha Gupta (India), Jade Forwood (Australia)

2:45pm - 5:10pm	<p>MS-10: Structural biology of eukaryotic immune systems Session Chair: Bostjan Kobe Session Chair: Savvas Savvides Invited: Tsan Sam Xiao (USA), Raul Olivier Martin (USA), Wen Song (Germany)</p>
2:45pm - 5:10pm	<p>MS-11: Ab initio powder structure analysis for polymorphism and phase transformation studies with pharmaceutical applications Session Chair: Martin U. Schmidt Session Chair: Fabia Gozzo Invited: Kenneth Harris (UK), Jim Kaduk (USA)</p>
2:45pm - 5:10pm	<p>MS-12: Quantum crystallographic studies on intra/inter-molecular interactions Session Chair: Anna Maria Makal Session Chair: Chérif F. Matta Invited: Jacob Overgaard (Denmark), Benoit Guillot (France)</p>
2:45pm - 5:10pm	<p>MS-13: Porous framework materials for gas adsorption/separation Session Chair: Angiolina Comotti Session Chair: Ryotaro Matsuda Invited: Michael Zaworotko (Ireland), Catharine Esterhuysen (South Africa)</p>
2:45pm - 5:10pm	<p>MS-14: Perovskites Session Chair: Chris Ling Session Chair: Philip Lightfoot Invited: James Rondinelli (USA), Joke Hadermann (Belgium)</p>
2:45pm - 5:10pm	<p>MS-16: Pre and post publication peer review of crystallographic data Session Chair: Mariusz Jaskolski Session Chair: Anthony Linden Invited: Stephen K. Burley (USA), Brian McMahon (UK)</p>
2:55pm - 5:55pm	<p>SF-2: Software Fayre 2 Session Chair: Martin Lutz http://www.cryst.chem.uu.nl/lutz/</p>
3:45pm - 5:15pm	<p>MS-15: Integrative methodologies for novel thin film structures Session Chair: David Babonneau Session Chair: Baerbel Krause Invited: Jolien Dendooven (Belgium), Byeongdu Lee (USA)</p>
5:10pm - 6:10pm Exhibition and poster area	<p>Afternoon break 1: Poster session A1, exhibition, coffee/tea</p>
6:10pm - 7:00pm	<p>KN-4: Crystal forms in pharmaceutical applications Session Chair: Marijana Đaković Susan Reutzel-Edens</p>
6:10pm - 7:00pm	<p>KN-5: State of the art understanding of diffraction from aperiodic crystals Session Chair: Ma. Louise Antonette Navarro De Las Peñas Uwe Grim</p>
6:10pm - 7:00pm	<p>KN-6: The Coronavirus Structural Task Force Session Chair: Marcin Nowotny Andrea Thorn</p>
7:15pm - 10:15pm	<p>IUCr: IUCr assembly Session Chair: Sven Lidin IUCr assembly 1</p>

Date: Monday, 16/Aug/2021

9:00am - 9:50am	KN-7: Crystalline sponge, metal-organic assembles Session Chair: Masaki Kawano Makoto Fujita
9:00am - 9:50am	KN-8: Order and disorder in metal-ion battery materials Session Chair: Elena Boldyreva Artem Abakumov
9:00am - 9:50am	KN-9: Electron crystallography of molecular crystals Session Chair: Václav Petříček Lukáš Palatinus
9:50am - 10:20am Exhibition and poster area	Morning break 2: Exhibition, posters, coffee/tea
10:20am - 12:45pm	MS-17: Automation in bio-crystallography: tools, perspectives and applications Session Chair: Santosh Panjikar Session Chair: Melanie Vollmar Invited: Katherine McAuley (UK), Jose Marquez (France)
10:20am - 12:45pm	MS-18a: Phase transitions in complex materials (structure and magnetism) I Session Chair: Yuichi Shimakawa Session Chair: Alexandra Gibbs Invited: Midori Amano Patino (Japan), Patrick Woodward (USA)
10:20am - 12:45pm	MS-19: Crystal structures of pharmaceutical and organic compounds from electron diffraction Session Chair: Ute Kolb Session Chair: Petr Brazda Invited: Enrico Mugnaioli (Italy), Brent Nannega (USA)
10:20am - 12:45pm	MS-20: Dynamic frameworks Session Chair: Christopher SUMBY Session Chair: Michael John Zaworotko Invited: Hoi Ri Moon (Republic of Korea), Yao Chen (China)
10:20am - 12:45pm	MS-21: Structure, modeling and properties of quasicrystals Session Chair: Michael Engel Session Chair: Cesar Baban Pay Gómez Invited: Tsunemoto Yamada (Japan), Priya Subramanian (UK)
10:20am - 12:45pm	MS-22: Methods and software developments for magnetic-structure analysis Session Chair: J. Manuel Perez-Mato Invited: Juan Rodriguez-Carvajal (Spain), Václav Petříček (Czech Republic)
10:20am - 12:45pm	MS-23: Ptychography: present and near future Session Chair: Manuel Guizar Sicaïros Session Chair: Julio Cesar da Silva Invited: Chris Jacobsen (USA), Julian Reinhardt (USA)
10:20am - 12:45pm	MS-24: Data-driven discovery in crystallography Session Chair: Olivier C. Gagné Session Chair: Anton Oliynyk Invited: Wenhao Sun (USA), Aria Mansouri Tehrani (Switzerland)
10:20am - 12:45pm	SF-3: Software Fayre 3 Session Chair: Martin Lutz http://www.cryst.chem.uu.nl/lutz/
12:45pm - 2:45pm Exhibition and poster area	Lunch 2: Exhibition, posters, lunches
12:45pm - 2:45pm	Meeting 1: ECA ECA council meeting 1
1:15pm - 2:45pm	CS-2: Commercial session 20 min company presentations
2:45pm - 5:10pm	MS-25: Structural biology against coronavirus/covid-1 Session Chair: Sarah EJ Bowman Session Chair: Lu Zhang Session Chair: Gianluca Santoni Invited: Xuhui Huang (China)
2:45pm - 5:10pm	MS-26: Solution scattering and combined techniques for biological systems, including

	component dynamics Session Chair: Frank Gabel Session Chair: Masaaki Sugiyama Invited: Mitsunori Ikeguchi (Japan), Anne Martel (France)
2:45pm - 5:10pm	MS-27: New trends in pharmaceutical materials Session Chair: Nikoletta B. Bathori Session Chair: Laszlo Fabian Invited: Tonglei Li (USA), Doris Braun (Austria)
2:45pm - 5:10pm	MS-28: Theory and practice of supramolecular synthons in crystal engineering Session Chair: Seiji Tsuzuki Session Chair: Alessia Bacchi Invited: Jindrich Fanfrlik (Czech Republic), Berta Gomez-Lor (Spain)
2:45pm - 5:10pm	MS-29: Texture, strain and structure in metals and ceramics Session Chair: David Rafaja Invited: Efthymios Polatidis (Switzerland), Jana Šmilauerová (Czech Republic)
2:45pm - 5:10pm	MS-30: Magnetic structures of novel and functional materials Session Chair: Virginie Simonet Session Chair: Václav Petříček Invited: Wei Tian (USA), Jonathan White (Switzerland)
2:45pm - 5:10pm	MS-31: Recent advances in instrumentation Session Chair: Ehrenfried Zschech Session Chair: Michele Cianci Invited: Wenbing Yun (USA), Andrew Thomson (France)
2:45pm - 5:10pm	MS-32: Recent advances in electron crystallography techniques Session Chair: Jim Ciston Session Chair: Mauro Gemmi Invited: Hongyj Xu (Sweden), Emanuela Liberti (UK)
2:45pm - 5:10pm	SMS-1: Exemplary practice in chemical, biological and materials database archiving Session Chair: Suzanna Ward Session Chair: Genji Kurisu Invited: Stacy Gates-Rector (USA), Annett Steudel (Austria)
5:10pm - 6:10pm Exhibition and poster area	Afternoon break 2: Poster session A2, exhibition, coffee/tea
6:10pm - 7:00pm	KN-10: Gjonnes medal lecture Session Chair: Louisa Meshi Ute Kolb, Sven Hovmöller
6:10pm - 7:00pm	KN-11: Structural hybrid methods to probe membrane transport nanomachines in pathogenic bacteria Session Chair: Julie Maria Jozefa Bouckaert Natalie Strynadka
6:10pm - 7:00pm	KN-12: Dithiadiazolyl radicals as building blocks for molecular magnetic materials Session Chair: Václav Petříček Delia Haynes
7:15pm - 10:15pm	IUCr-2: IUCr assembly Session Chair: Sven Lidin IUCr assembly 2

Date: Tuesday, 17/Aug/2021

9:00am - 9:50am	KN-13: Time resolved macromolecular crystallography Session Chair: Alice Vrielink Arwen R Pearson
9:00am - 9:50am	KN-14: Structural flexibility and disorder in functional materials Session Chair: Brendan Kennedy Andrew Goodwin
9:00am - 9:50am	KN-15: Quantum crystallography and spintronic materials Session Chair: Krzysztof Wozniak Piero Macchi
9:50am - 10:20am Exhibition and poster area	Morning break 3: Exhibition, posters, coffee/tea
10:20am - 12:45pm	MS-33: CryoEM for macromolecules - from single particles to microcrystals Session Chair: Jan Pieter Abrahams Session Chair: Jiri Novacek Invited: Nenad Ban (Switzerland), Dimple Karia (Netherlands)
10:20am - 12:45pm	MS-34a: Structural biology of enzymes, mechanism and regulation Session Chair: Mirjam Czjzek Invited: Liang Wu (UK), Orsolya Barabas (Germany)
10:20am - 12:45pm	MS-35: Polymorphism and structural transformation of organic crystals from synthesis to characterization Session Chair: Kenneth D. M. Harris Session Chair: Doris E. Braun Invited: David Bryce (Canada), Franziska Emmerling (Germany)
10:20am - 12:45pm	MS-36: Generalizations of crystallographic groups and their applications Session Chair: Gregory L McColm Session Chair: Eden Delight Miro Invited: Pavel Kalouguine (France), Martin Cramer Pedersen (Denmark)
10:20am - 12:45pm	MS-37: Total scattering Session Chair: Pierre Bordet Session Chair: Emil Bozin Invited: Stephan Rosenkranz (USA), Bo Brummerstedt Iversen (Denmark)
10:20am - 12:45pm	MS-38: Structural, electronic and magnetic ordering: From fundamental physics to functionality Session Chair: Javier Sanchez-Benitez Session Chair: Ovidiu Garlea Invited: Steve Nagler (USA), Mark Senn (UK)
10:20am - 12:45pm	MS-39: Quantum crystallography in materials science Session Chair: Simon Grabowsky Session Chair: Jean-Michel Gillet Invited: Renecca Scatena (UK), Cherif Matta (Canada)
10:20am - 12:45pm	MS-40: New applications of coherent scattering Session Chair: Ian Robinson Session Chair: Christian Gutt Invited: Johanned Ihli (Switzerland), Foivos Perakis (Sweden)
10:20am - 12:45pm	SMS-2: Online crystallography: Tools, apps and web services Session Chair: Eugene Krissinel Session Chair: Christian Bertram Hübschle Invited: Mois Ilia Aroyo (Spain), Victor Lamzin (Germany)
12:45pm - 2:45pm	ECA-ECM: ECM programme committees ECM programme committee meetings -Versaille,Padova
12:45pm - 2:45pm Exhibition and poster area	Lunch 3: Exhibition, posters, lunches
1:15pm - 2:45pm	CS-3: Commercial session 20 min company presentations
3:00pm - 3:50pm	PL-1: How data have revealed the structural universe Helen Berman
3:50pm - 4:40pm	Bragg: Braggs prize lecture

4:40pm - 5:40pm Exhibition and poster area	Afternoon break 3: Poster session B1, exhibition, coffee/tea
5:40pm - 6:30pm	PL-2 Clare Grey
6:30pm - 7:15pm Exhibition and poster area	Refreshment: Refreshment
7:15pm - 8:45pm	Cultural programme: Concert

Date: Wednesday, 18/Aug/2021

9:00am - 9:50am	KN-16: MicroED: conception, practice and future opportunities Session Chair: Louisa Meshi Tamir Gonen
9:00am - 9:50am	KN-17: Electron density, and its interplay with the energy and properties of molecules and solids Session Chair: Catharine Esterhuysen Julia Contreras-Garcia
9:00am - 9:50am	KN-18: In-situ and In-operando diffraction Studies of Li Ion Battery Electrodes Session Chair: Radovan Cerny Gwenaelle Rousse
9:50am - 10:20am Exhibition and poster area	Morning break 4: Exhibition, posters, coffee/tea
10:20am - 12:45pm	MS-41: Macromolecular machines and hybrid methods to crystallography Session Chair: Michael Landsberg Session Chair: Dmitry Svergun Invited: Kristina Djinovic-Carugo (Austria), Tanmay Bharat (India)
10:20am - 12:45pm	MS-42: Novel techniques and insights into in vitro and in situ crystallisation for X-ray and electron diffraction. Session Chair: Lars Redecke Session Chair: Fasseli Coulibaly Invited: Haruki Hasegawa (USA), Alexandra Ros (USA)
10:20am - 12:45pm	MS-43: Solid state reactions and dynamics Session Chair: Franziska Emmerling Session Chair: Javier Marti-Rujas Invited: Hiroyoshi Ohtsu (Japan), Paolo Pio Mazzeo (Italy)
10:20am - 12:45pm	MS-44: Beyond pure point diffraction: Theory and application of diffuse scattering Session Chair: Nicolae Strungaru Session Chair: Uwe Grimm Invited: Chrizaldi Neil Manibo (Germany), Ella Mara Schmidt (Germany)
10:20am - 12:45pm	MS-45: Frustrated magnetic order and emerging science Session Chair: Romain Sibille Session Chair: Geetha Balakrishnan Invited: Beauvois Ketty (France), Nicolas Gauthier (USA)
10:20am - 12:45pm	MS-46: In-situ and in operando studies of battery materials Session Chair: Vanessa Kate Peterson Session Chair: Claire Villeveille Invited: Karena Chapman (USA), Sandrine Lyonnard (France)
10:20am - 12:45pm	MS-47a: Nanocrystalline materials I Session Chair: Cinzia Giannini Session Chair: Jinong Zhu Invited: Junliang Sun (China), Ulf Olsson (Sweden)
10:20am - 12:45pm	MS-48: Combination of X-rays and electrons for structure characterization Session Chair: Joke Hadermann Session Chair: Junliang Sun Invited: Stef Smeets (Netherlands), Tatiana Gorelik (Germany)
10:20am - 12:45pm	SF-4: Software Fayre 4 Session Chair: Martin Lutz http://www.cryst.chem.uu.nl/lutz/
12:45pm - 2:45pm Exhibition and poster area	Lunch 4: Exhibition, posters, lunches
12:45pm - 2:45pm	Meeting 2: ECA ECA council meeting 1
12:45pm - 2:45pm Exhibition and poster area	Lunch 5: Posters, lunches
1:15pm - 2:45pm	CS-4: Commercial session 20 min company presentations
2:45pm - 5:10pm	MS-49: Protein design and engineering

	<p>Session Chair: Charlotte Uetrecht Session Chair: Sheena McGowan Invited: Elizabeth M.J. Gillam (Australia), Mauri Kostianen (Finland)</p>
2:45pm - 5:10pm	<p>MS-51: Molecular magnets and metal-organic frameworks including quantum crystallography approaches Session Chair: Jozef Kozisek Session Chair: Verónica Paredes-García Invited: Ivan Němec (Czech Republic), Andrade Malaspina (France)</p>
2:45pm - 5:10pm	<p>MS-52: Combining X-ray diffraction and spectroscopy to characterise materials Session Chair: Carlo Meneghini Session Chair: Siebert Schmid Invited: Ilaria Carlomagno (Italy), Marco Giorgetti (Italy)</p>
2:45pm - 5:10pm	<p>MS-53: Function and application of porous crystals Session Chair: Karena Chapman Session Chair: Fernando Uribe-Romo</p>
2:45pm - 5:10pm	<p>MS-54: Materials for energy conversion and storage Session Chair: Jean-Marc Joubert Session Chair: Stefan Adams Invited: Yaroslav Filinchuk (Belgium), Kent Griffith (USA)</p>
2:45pm - 5:10pm	<p>MS-55(47b): Nanocrystalline materials II Session Chair: Cinzia Giannini Session Chair: Jinong Zhu</p>
2:45pm - 5:10pm	<p>MS-56: Analysis of the fine structure in electron diffraction data Session Chair: Tatiana Gorelik Session Chair: Xiaodong Zou Invited: Paul Voyles (USA), Cheuk-Wai Tai (Sweden)</p>
2:45pm - 5:10pm	<p>SMS-3: Using crystallography for education during the pandemic Session Chair: Oluwatoyin Asojo Invited: Karsten Theis (USA)</p>
2:55pm - 5:55pm	<p>SF-5: Software Fayre 5 Session Chair: Martin Lutz http://www.cryst.chem.uu.nl/lutz/</p>
5:10pm - 6:10pm Exhibition and poster area	<p>Afternoon break 4: Poster session B2, exhibition, coffee/tea</p>
6:10pm - 7:00pm	<p>KN-19: How limitless antibodies are generated by V(D)J recombination Session Chair: Marcin Nowotny Wei Yang</p>
6:10pm - 7:00pm	<p>KN-20: Identification of secondary phase structure using 4D Precession Electron Diffraction Session Chair: Louisa Meshi Edgar Rauch</p>
6:10pm - 7:00pm	<p>KN-21: X-ray absorption spectroscopy and materials science: recent advances Session Chair: Giuliana Aquilanti Federico Boscherini</p>

Date: Thursday, 19/Aug/2021

9:00am - 9:50am	KN-22
9:00am - 9:50am	KN-23: Novel insights on biomineralization using x-rays and optical coherent diffraction based imaging Session Chair: Sakura Pascarelli Virginie Chamard
9:00am - 9:50am	KN-24: Record High superconductivity in sodalite-like rare-earth hydrides stabilized at high pressures Session Chair: Arthur Haozhe Liu Yanming Ma
9:50am - 10:20am Exhibition and poster area	Morning break 5: Posters, coffee/tea
10:20am - 12:45pm	MS-57: Neutron scattering - sources, applications Session Chair: Matthew Paul Blakeley Session Chair: Flora Meilleur Session Chair: Esko Oksanen Invited: Gloria Borgstahl (USA), Svetlana Antonyuk (UK)
10:20am - 12:45pm	MS-58: Ultra-high resolution macromolecular crystallography and quantum biocrystallography Comments Session Chair: Christian Jelsch Session Chair: Alexander Wlodawer Invited: Paulina Dominiak (Poland), Maciej Kubicki (Poland)
10:20am - 12:45pm	MS-59: Crystal chemistry with emerging technology I Session Chair: Consiglia Tedesco Session Chair: Toru Asahi Invited: Katharina Fromm (Switzerland), Sota Sato (Japan)
10:20am - 12:45pm	MS-60: Composite and incommensurate modulated crystals: structural and physical properties Session Chair: Sylvain Ravy Session Chair: Sander van Smaalen Invited: Stephan J. Skinner (UK), Vincent Jacques (France)
10:20am - 12:45pm	MS-61: Magnetic structures at extreme conditions and in extreme samples Session Chair: Angel M. Arevalo-Lopez Session Chair: Andrzej Katrusiak Invited: Elena Solana-Madruga (UK), Dawid Pinkowicz (Poland)
10:20am - 12:45pm	MS-62: The mineral/life interface - prebiotic chemistry, biomineralization, advanced biomimetic materials Session Chair: Juan Manuel Garcia-Ruiz Session Chair: Giuseppe Falini Invited: Boaz Pokroy (Israel), Abel Moreno (Mexico)
10:20am - 12:45pm	MS-63: Catalysis: functionalized materials studied by XRD and XAFS Session Chair: Valérie Briois Session Chair: Andreas Roodt Invited: Elisa Borfecchia (Italy), Ola F Wendt (Sweden)
10:20am - 12:45pm	MS-64: In-situ and time resolved electron crystallography Session Chair: Andrew Alexander Stewart Session Chair: Eva Olsson Invited: David Flannigan (USA), Maria Batuk (Belgium)
10:20am - 12:45pm	SF-6: Software Fayre 6 Session Chair: Martin Lutz http://www.cryst.chem.uu.nl/lutz/
1:15pm - 2:45pm	CS-5: Commercial session 20 min company presentations
2:45pm - 5:10pm	MS-65: Graphs, tilings and crystal structures Session Chair: Mark Loyola Session Chair: Bernd Souvignier Invited: Vladislav A. Blatov (Russia), Jean-Guillaume Eon (Brazil)
2:45pm - 5:10pm	MS-66: Integrative structural biology: The next 50 years of the Protein Data Bank Session Chair: Stephen K. Burley Session Chair: Dina Schneidman Invited: Andrej Sali (USA), Fei Xu (China)

2:45pm - 5:10pm	<p>MS-67: Crystallization mechanisms of small molecule systems Session Chair: Duane Choquesillo-Lazarte Invited: Ian Rosbottom (UK), Aurora Cruz-Cabeza (UK)</p>
2:45pm - 5:10pm	<p>MS-68: Symmetry aspects of magnetic order and magnetic properties Session Chair: Mois Iliá Aroyo Session Chair: Margarida Henriques Invited: Laura Chaix (France), Fabio Orlandi (UK)</p>
2:45pm - 5:10pm	<p>MS-69a: Complex crystal structures - chemical crystallography Session Chair: Marie Colmont Session Chair: Sergey V. Krivovichev</p>
2:45pm - 5:10pm	<p>MS-70: Matter at extreme conditions at SR and XFEL: complementarity of spectroscopy and diffraction Session Chair: Angelika Dorothea Rosa Session Chair: Ulf Zastra Invited: Virginia Monteseguro (Spain, ESRF), Emma McBride (USA, SLAC)</p>
2:45pm - 5:10pm	<p>MS-71a: Disordered materials: spectroscopic and scattering techniques I Session Chair: Simon Billinge Session Chair: Angela Trapananti Invited: Takeshi Egami (USA), Shinya Hosokawa (Japan)</p>
2:45pm - 5:10pm	<p>MS-72: New methods and strategies in NMR crystallography - in Honour of Francis Taulelle Session Chair: Martin Dracinsky Session Chair: David Bryce Invited: Sharon Ashbrook (UK), Lyndon Emsley (Switzerland)</p>
2:55pm - 5:55pm	<p>SF-7: Software Fayre 7 Session Chair: Martin Lutz http://www.cryst.chem.uu.nl/lutz/</p>
5:10pm - 6:10pm Exhibition and poster area	<p>Afternoon break 5: Poster session C1, coffee/tea</p>
6:10pm - 7:00pm	<p>KN-25: A Crystallographic Snapshot of SARS-CoV-2 Main Protease Maturation Process and the Discovery of Inhibitors Session Chair: Julie Maria Jozefa Bouckaert Glaucius Oliva</p>
6:10pm - 7:00pm	<p>KN-26: Complexity in crystals and minerals Session Chair: Patrick H.J. Mercier Sergey Krivovichev</p>
6:10pm - 7:00pm	<p>KN-27: Crystallography and cultural heritage - On beauty, science and passion Session Chair: Jose Miguel Delgado Gilberto Artioli</p>
7:15pm - 10:15pm	<p>IUCr-3: IUCr assembly Session Chair: Sven Lidin IUCr assembly 3</p>

Date: Friday, 20/Aug/2021

9:00am - 9:50am	KN-28: Structure guided inhibitor discovery targeting a membrane receptor involved in atherosclerosis Session Chair: Alice Vrielink Arockiasamy Arulandu
9:00am - 9:50am	KN-29: 4th generation SR and XFEL facilities: new era in crystallography and material science Aleksandr Blagov
9:00am - 9:50am	KN-30: Mechanical properties of crystals Malla Reddy
9:50am - 10:20am Exhibition and poster area	Morning break 6: Posters, coffee/tea
10:20am - 12:45pm	MS-73: Machine learning in biological and structural sciences Session Chair: Rita Giordano Session Chair: Harold Roger Powell Invited: Melanie Vollmar (UK), Sergei Grudinin (France)
10:20am - 12:45pm	MS-74: Structural biology of receptors, signaling and membrane proteins Session Chair: SUSAN KAY BUCHANAN Session Chair: Michael Parker Invited: Robert Keenan (USA), Isabel Moraes (UK)
10:20am - 12:45pm	MS-75: Small- and Wide-Angle Scattering for industrial materials far from equilibrium Session Chair: Jan Ilavsky Session Chair: Semra IDE Invited: Masato Ohnuma (Japan), Elliot Paul Gilbert (Australia)
10:20am - 12:45pm	MS-76(59b): Crystal chemistry with emerging technology II Session Chair: Consiglia Tedesco Session Chair: Toru Asahi
10:20am - 12:45pm	MS-77(71b): Disordered materials: spectroscopic and scattering techniques II Session Chair: Simon Billinge Session Chair: Angela Trapananti Invited: Lars G. M. Pettersson (Sweden), Maxwell Terban (Germany)
10:20am - 12:45pm	MS-78: Science meets art: X-ray spectrometry and X-ray diffraction in art and archaeology Session Chair: Gilberto Artioli Session Chair: Sebastian Bette Invited: Katrien Keune (Netherlands), Christoph Berthold (Germany)
10:20am - 12:45pm	MS-79(69b): Complex structures of minerals and inorganic materials Session Chair: Marie Colmont Session Chair: Sergey V. Krivovichev
10:20am - 12:45pm	MS-80: 4th generation SR and XFEL Facilities Session Chair: Makina Yabashi Session Chair: Sofia Diaz-Moreno Invited: Matt Newville (USA), Jean Susini (France)
10:20am - 12:45pm	SMS-4: Session in the memory of An-Pang Tsai: from quasicrystals to catalysis Session Chair: Marc de Boissieu Session Chair: Yasushi Ishii
12:45pm - 2:45pm	ECA-3: ECA EC meeting with SIGS ECA EC meeting with SIG representative
12:45pm - 2:45pm Exhibition and poster area	Lunch 6: Posters, lunches
1:15pm - 2:45pm	CS-6: Commercial session 20 min company presentations
2:45pm - 5:10pm	MS-81: Nucleic acids and binding proteins structure and function Session Chair: Stephen Neidle Session Chair: Charles Bond Invited: Millie Georgiadis (USA), Liliya Yatsunyk (USA)
2:45pm - 5:10pm	MS-82: Handling of big data in crystallography Session Chair: Wladek Minor Session Chair: Brinda Vallat
2:45pm - 5:10pm	MS-83: High pressure crystallography

	<p>Session Chair: Lars Ehm Session Chair: Jon Henry Eggert Session Chair: Vitali Prakapenka Session Chair: Przemyslaw Dera Invited: Norimasa Ozaki (Japan), Rachel Husband (Germany)</p>
2:45pm - 5:10pm	<p>MS-85: Science meets art: Crystallography and cultural heritage Session Chair: Alicja Rafalska-Lasocha Session Chair: Petr Bezdzicka Invited: Koen Janssens (Belgium), Sebastian Bette (Germany)</p>
2:45pm - 5:10pm	<p>MS-86: Modular structure of inorganic and mineral compounds Session Chair: Isabella Pignatelli Session Chair: Berthold Stöger Invited: Olivier Perez (France), Marie Colmont (France)</p>
2:45pm - 5:10pm	<p>MS-87: Topological materials Session Chair: Catherine Pappas Session Chair: Yugui Yao Session Chair: Wenhui Duan Session Chair: Avadh B. Saxena Invited: hr. Pfeleiderer (Germany), Tomasz Dietl (Poland), Xiang Li (China)</p>
2:45pm - 5:10pm	<p>MS-88: Quantum crystallography research Session Chair: Yu-Sheng Chen Session Chair: Katarzyna N. Jarzemska Invited: Sophie E. Canton (Hungary), Simon Grabowsky (Switzerland)</p>
2:45pm - 5:10pm	<p>SMS-6: Spectroscopy applied to electrochemistry: operando studies Session Chair: Jasper Rikkert Plaisier Session Chair: Dibyendu Bhattacharyya Invited: Moniek Tromp (The Netherlands), Mahalingam Balasubramanian (USA)</p>
2:55pm - 5:55pm	<p>SF-8: Software Fayre 8 Session Chair: Martin Lutz http://www.cryst.chem.uu.nl/lutz/</p>
2:55pm - 5:55pm	<p>SMS-5: Advances in data and model validation in biomolecular Small-Angle Scattering: Impacts on data and meta-data recording and data archiving Session Chair: Javier Perez Invited: Dina Schneidman (Israel), Thomas Grant (USA)</p>
5:10pm - 6:10pm Exhibition and poster area	<p>Afternoon break 6: Poster session C2, coffee/tea</p>
6:10pm - 7:00pm	<p>KN-31: The contribution of crystallography to new vaccine formulations Session Chair: Graciela Carlota Díaz de Delgado Marcia Fantini</p>
6:10pm - 7:00pm	<p>KN-32 Session Chair: Thomas Proffen Ken Andersen</p>
6:10pm - 7:00pm	<p>KN-33: The crystal and the rose: On the impact of crystals and crystallography in art and mind Session Chair: Abel MORENO Juan Manuel Garcia-Ruiz</p>
8:00pm - 11:00pm National House	<p>Dinner: Conference dinner extra fee</p>

Date: Saturday, 21/Aug/2021

9:00am - 9:50am	KN-34: Fabrication and Characterization of Inhomogeneity-free Polymer Gels Session Chair: Marijana Đaković Mitsushiro Shibayama
9:00am - 9:50am	KN-35: The Science of Symmetry Breaking Session Chair: Oksana Zaharko Harold Stokes
9:00am - 9:50am	KN-36: Metadata and checkCIF for raw diffraction data in realising ultimate crystallographic objectivity Session Chair: John Richard Helliwell Loes Kroon-Batenburg
9:50am - 10:20am Exhibition and poster area	Morning break 7: Coffee/tea
10:20am - 12:45pm	MS-89: Fragment Screening, LCP, and Automation Session Chair: Alice Douangamath Session Chair: Lisa J. Keefe Invited: Steve Soisson (USA), Martin Noble (UK)
10:20am - 12:45pm	MS-90: Structure solution and poorly crystalline materials Session Chair: Angela Altomare Invited: Martin Schmidt (Germany), Katharine Page (USA)
10:20am - 12:45pm	MS-91: Time-resolved phase evolution, interaction & crystallization in soft matter: Integrative approaches Session Chair: Mitsushiro Shibayama Session Chair: Jrjeng Ruan Invited: Julia Kornfield (USA), Christine M. Papadakis (Germany)
10:20am - 12:45pm	MS-92 (34b): Structural biology of enzymes, mechanism and regulation II Session Chair: Mirjam Czjzek Session Chair: Beata G. Vertessy
10:20am - 12:45pm	MS-93: Non-covalent interactions in crystal engineering I Session Chair: Giuseppe Resnati Session Chair: Petra Bombicz Invited: Deepak Chopra (India), Karah Knope (USA)
10:20am - 12:45pm	MS-94: Organic minerals, metal-organic frameworks, and metal-oxygen clusters: the emergent interface of geochemistry and crystal engineering Session Chair: Igor Huskić Session Chair: Tomoji Ozeki Invited: Helen Maynard-Casely (Australia), Ulrich Kortz (Germany)
10:20am - 12:45pm	MS-95: Advanced methods for analysis of XAFS and crystallographic data Session Chair: Marco Giorgetti Session Chair: Paula Macarena Abdala Invited: Paola D'angelo (Italy), Rocco Caliendo (Italy)
10:20am - 12:45pm	MS-96: Crystallography schools to promote interdisciplinarity in science Session Chair: Alice Brink Session Chair: Serena Chiara Tarantino Invited: Diego German Lamas (Argentina), Marielle Yasmine Agbahoungbata (Benin)
10:20am - 12:45pm	SMS-7: Hydrogen rich compounds: design, properties & phase transitions at high pressures Session Chair: Artem R Oganov Session Chair: Alexander Goncharov Invited: Chris J. Pickard (UK), Dmitry Semenok (Russia)
12:45pm - 2:45pm Exhibition and poster area	Lunch 7: Lunches
2:45pm - 5:10pm	MS-100: Stimuli-responsive crystalline compounds Session Chair: Chiara Massera Session Chair: Ivan Halasz Invited: Tomce Runcevski (USA), Helena Shepherd (UK)
2:45pm - 5:10pm	MS-102: Crystallography using large volume presses and diamond anvil cells Session Chair: Shanti Deemyad Session Chair: Ronald MILETICH Invited: Natalia Dubrovinskaia (Germany), Siddharth Saxena (UK)
2:45pm - 5:10pm	MS-103: XAS and crystallography allied for geomaterials and environmental problems

	<p>Session Chair: J. Fred Mosselmans Session Chair: Annalisa Martucci Invited: Giuseppe Cruciani (Italy), Georgia Cametti (Switzerland)</p>
2:45pm - 5:10pm	<p>MS-104: Diffraction imaging, grain mapping in materials and art Session Chair: Jonathan Paul Wright Session Chair: Sine Larsen Invited: Ashley Bucsek (USA), Frederik Vanmeert (Belgium)</p>
2:45pm - 5:10pm	<p>MS-97: New methods to fight the pandemic Session Chair: Jane Shelby Richardson Session Chair: Nicholas Mark Pearce Invited: Jasmine Young (USA), Tristan Croll (UK)</p>
2:45pm - 5:10pm	<p>MS-98: 2D type crystals and their heterostructures Session Chair: Matteo Bosi Session Chair: Adela Rodriguez-Romero Invited: Eli Sutter (USA), Xinliang Feng (Germany)</p>
2:45pm - 5:10pm	<p>MS-99: Non-covalent interactions in crystal engineering II Session Chair: Giuseppe Resnati Session Chair: Petra Bombicz Invited: Andrea Pizzi (Italy), Christian Jelsch (France)</p>
2:55pm - 5:10pm	<p>MS-101 (18b): Phase transitions in complex materials (structure and magnetism) II Session Chair: Yuichi Shimakawa Session Chair: Alexandra Gibbs</p>
5:10pm - 5:40pm Exhibition and poster area	Afternoon break 7: Coffee/tea
5:40pm - 6:30pm	<p>PL-3: The structural biology of pathogenic amyloid fibrils David Eisenberg</p>
6:30pm - 7:30pm	Closing ceremony: Poster prizes, closing

Date: Sunday, 22/Aug/2021

8:00am - 10:00pm	Train trip Pilsen: Plzeň Exact time of the trip will be determined. Prague - Pilsen, excursion in brewery, lunch, Pilsen - Prague. Alternative to the trip to Český Krumlov.
8:00am - 10:00pm	Train trip: Český Krumlov Train trip Prague - Český Krumlov - Prague

Date: Monday, 23/Aug/2021

	Poster - Photochemistry: Solid state photo chemistry Day and time of the session to be determined.
	Poster - Art: Crystallography in art and archaeology Day and time of the session to be determined.
	Poster - Automation in bio: Automation in biocrystallography Day and time of the session to be determined.
	Poster - Biocrystallography: Macromolecular and biological crystallography Day and time of the session to be determined.
	Poster - Bioinformatics: Structural bioinformatics Session Chair: Jiri Cerny Session Chair: Bohdan Schneider Day and time of the session to be determined.
	Poster - Biomineralization: Biomineralization, advanced biomimetic materials Day and time of the session to be determined.
	Poster - Chemical: Chemical crystallography Day and time of the session to be determined.
	Poster - CryoEM: Cryo-EM Session Chair: Jose-Maria Carazo Session Chair: Jiri Novacek Day and time of the session to be determined.
	Poster - Crystal engineering: Crystal engineering, theory and practice Day and time of the session to be determined.
	Poster - Crystallization: Theoretical crystallography Day and time of the session to be determined.
	Poster - Data: Crystallographic data Day and time of the session to be determined.
	Poster - Disordered: Disordered materials Session Chair: Simon Billinge Session Chair: Angela Trapananti Day and time of the session to be determined.
	Poster - Drug design: Crystallographic data Day and time of the session to be determined.
	Poster - Electron: Electron crystallography Day and time of the session to be determined.
	Poster - Energy: Materials for energy conversion and storage Session Chair: Stefan Adams Session Chair: Jean-Marc Joubert Day and time of the session to be determined.
	Poster - Enzymes: Structural biology of enzymes Day and time of the session to be determined.
	Poster - Films: Crystallographic analysis of thin films and surfaces Day and time of the session to be determined.
	Poster - General: General interest Day and time of the session to be determined.
	Poster - High Pressure: High Pressure Crystallography Day and time of the session to be determined.
	Poster - Hot structures: Hot structures of biological importance Day and time of the session to be determined.
	Poster - Industry: Crystallography in industry and applied sciences Day and time of the session to be determined.
	Poster - Instrumentation: Advances in instrumentation Day and time of the session to be determined.

	<p>Poster - Magnetism: Magnetic structures Day and time of the session to be determined.</p>
	<p>Poster - Minerals: Complex structures of minerals and inorganic materials Session Chair: Marie Colmont Session Chair: Sergey V. Krivovichev Session Chair: Milan Rieder Day and time of the session to be determined.</p>
	<p>Poster - Modular: Modular structure of inorganic and mineral compounds Day and time of the session to be determined.</p>
	<p>Poster - Modulated: Composite and Incommensurate Modulated Crystals Session Chair: Sander van Smaalen Session Chair: Sylvain Ravy Day and time of the session to be determined.</p>
	<p>Poster - MOF: Metal-organic frameworks Day and time of the session to be determined.</p>
	<p>Poster - Nano: Nanomaterials Session Chair: Cinzia Giannini Session Chair: Jinong Zhu Day and time of the session to be determined.</p>
	<p>Poster - Neutrons: Neutron scattering Session Chair: Jiri Kulda Day and time of the session to be determined.</p>
	<p>Poster - NMR: NMR crystallography Session Chair: David Bryce Session Chair: Martin Dracinsky Day and time of the session to be determined.</p>
	<p>Poster - Non-covalent: Non-covalent interactions in crystal engineering Session Chair: Petra Bombicz Session Chair: Giuseppe Resnati Day and time of the session to be determined.</p>
	<p>Poster - Perovskites: Perovskites Session Chair: Philip Lightfoot Session Chair: Chris Ling Date and time of the session to be determined.</p>
	<p>Poster - Pharmaceutical: Pharmaceutical materials Date and time of the session to be determined.</p>
	<p>Poster - Phase transitions: Structure and phase transitions in advanced materials Date and time of the session to be determined.</p>
	<p>Poster - Physics: Solid state photo chemistry Date and time of the session to be determined.</p>
	<p>Poster - Polymorphism: Polymorphism Session Chair: Doris E. Braun Session Chair: Kenneth D. M. Harris Date and time of the session to be determined.</p>
	<p>Poster - Porous: Porous materials Date and time of the session to be determined.</p>
	<p>Poster - Powder: Powder diffraction Date and time of the session to be determined.</p>
	<p>Poster - Protein design: Protein design and engineering Date and time of the session to be determined.</p>
	<p>Poster - Ptychography: Ptychography, imaging, coherent scattering Date and time of the session to be determined.</p>
	<p>Poster - Quantum: Quantum crystallography Date and time of the session to be determined.</p>
	<p>Poster - Receptors: Structural biology of receptors, membrane proteins Date and time of the session to be determined.</p>
	<p>Poster - SAXS: SAXS, SANS Session Chair: Semra IDE Session Chair: Jan Ilavsky Date and time of the session to be determined.</p>

	<p>Poster - Solid state: Solid state reactions and dynamics Date and time of the session to be determined.</p>
	<p>Poster - Solution scattering: Structural biology of receptors, membrane proteins Date and time of the session to be determined.</p>
	<p>Poster - Spectroscopy: Combining X-Ray Diffraction and Spectroscopy to Characterise Materials Session Chair: Carlo Meneghini Session Chair: Siegbert Schmid Date and time of the session to be determined.</p>
	<p>Poster - Structure prediction: Crystal structure prediction Date and time of the session to be determined.</p>
	<p>Poster - Supramolecular: Theory and practice of supramolecular synthons in crystal engineering Date and time of the session to be determined.</p>
	<p>Poster - Synchrotron and XFEL: Synchrotron and XFEL facilities Date and time of the session to be determined.</p>
	<p>Poster - Texture, defects: Texture, strain, stress, real structure Session Chair: David Rafaja Date and time of the session to be determined.</p>
	<p>Poster - Theory: Theoretical crystallography Date and time of the session to be determined.</p>
	<p>Poster - Time-resolved: Time resolved phase evolution, interaction and crystallization in soft matter Date and time of the session to be determined.</p>
	<p>Poster - Total: Total scattering Session Chair: Emil Bozin Session Chair: Pierre Bordet Date and time of the session to be determined.</p>
	<p>Poster - Viruses: Structural biology of viruses Date and time of the session to be determined.</p>
	<p>Poster - XAFS: XAFS Date and time of the session to be determined.</p>

Date: Wednesday, 01/Sept/2021

2:00pm - 8:00pm	School - Computing: Crystallographic Computing School Session Chair: Martin Lutz Session Chair: Claudia Millán
virtual	

2:00pm - 8:00pm	School - ePDF: School on electron PDF (pair-distribution function) Session Chair: Tatiana Gorelik virtual meeting
virtual	

Date: Thursday, 02/Sept/2021

<p>2:00pm - 8:00pm</p> <p>virtual</p>	<p>School - Computing 2: Crystallographic Computing School Session Chair: Martin Lutz Session Chair: Claudia Millán</p>
<p>2:00pm - 8:00pm</p>	<p>School - ePDF 2: School on electron PDF (pair-distribution function) Session Chair: Tatiana Gorelik virtual meeting</p>

Date: Friday, 03/Sept/2021

2:00pm - 8:00pm

virtual

School - Computing 3: Crystallographic Computing School

Session Chair: **Martin Lutz**

Session Chair: **Claudia Millán**