

FIRST AUTHOR'S LAST NAME	FIRST AUTHOR'S FIRST NAME	POSTER ID	OTHER AUTHORS' NAMES	TITLE	FLOOR	PANEL NR.	DAY	SESSION
Zheng	Shao-Liang	4		Addressing Crystallography Misconceptions for Chemistry Students	THIRD FLOOR	134	27 August, Tue.	MS41 - Approaches and tools for learning crystallography efficiently and avoiding misconceptions
Nemec	Ivan	5		Interplay of Halogen Bonding and Semi-Coordination in Co(II) Single-Ion Magnets	SECOND FLOOR	104	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Boucherabine	Djihed	6		Copper complexes of new unsymmetrically NNOO ligands: X- ray structure, NLO properties, catalytic oxidation and bromoperoxidase activities	THIRD FLOOR	115	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Singh	Charandeep	7	Krishan Gopal Thakur	Structural insights into Polymorphic toxin -Immunity pair system of Bacillus subtilis	GROUND FLOOR	1	27 August, Tue.	MS02 - Hot structures
Hinuma	Yoyo	10		On the effectiveness of first-year-of-university math and somewhat brute force computing when developing new methods in crystallography	SECOND FLOOR	104	29 August, Thur.	MS38
Blaaha	Jan	12		Efficient enrichment of in cellulose grown protein crystals	FIRST FLOOR	34	28 August, Wed.	MS10
Moeck	Peter	13		Symmetries and pseudo-symmetries in a sophisticated piece of graphic art and beyond	THIRD FLOOR	117	29 August, Thur.	MS36
Shaw Stewart	Patrick	14		Sample preparation for routine and advanced structural biology ECM	GROUND FLOOR	5	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
Baldock	Peter	15	Stefan Kolek; Patrick Shaw Stewart; Jack Stubbs	Sample preparation for routine and advanced structural biology, including serial data collection and microED	GROUND FLOOR	6	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
Lutz	Martin	16		Pseudo-centrosymmetry can confuse automatic space group determination	THIRD FLOOR	127	29 August, Thur.	MS39
Zhao	Yongsheng	19		PRESSURE INDUCED SUPERCONDUCTOR IN Rb2Mo6Se6	THIRD FLOOR	155	28 August, Wed.	MS12
Bae	Euiyoung	20	Hyejin Oh	Crystal structure of GajB protein in Gabija anti-phage defense	FIRST FLOOR	31	27 August, Tue.	MS6 - Structural studies in Enzymology
Siebert	Alistair	21		HeXI: The High-energy Electron Xtallography Instrument at Diamond Light Source	FIRST FLOOR	53	28 August, Wed.	MS16
Bhattacharya	Suman	22		Multicomponent crystals of sulfamic acid with amino acids as alternative piezoelectric / NLO materials	THIRD FLOOR	116	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Yoon	Hye-Jin	23		The effect of R518W mutation on the function of NPC1 cholesterol transport: Molecular dynamics simulation study	FIRST FLOOR	32	27 August, Tue.	MS6 - Structural studies in Enzymology
Levendis	Demetrius	24		Crystallographic study of NaClO3 and NaBrO3: addressing misconceptions about chirality, absolute configuration, and optical rotation	FIRST FLOOR	98	27 August, Tue.	MS26 - Chirality: Meeting point of crystallography, chemistry and topology
Kherfi	Hamza	26		Different Hydrogen-bond networks in two 1D bimetallic oxalate compounds: ACr(C2O4)2(H2O)4 (A = Li, Na)	SECOND FLOOR	105	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Ignatev	Vladislav	28	Paulina Dominiak	The influence of wave function's basis set on the fit of multipole model to wave function	FIRST FLOOR	45	28 August, Wed.	MS11
Rogan	Jelena	29		Crystal structure and computational study of cobalt(II) coordination polymer with 2,2'-dipyridylamine and anion of isophthalic acid	THIRD FLOOR	141	27 August, Tue.	MS29 - Structural characterization in Functional materials
Radovanović	Lidija	30		Crystallographic and quantum chemical studies of xanthen-1,8(2H)-dione derivatives	THIRD FLOOR	142	27 August, Tue.	MS29 - Structural characterization in Functional materials
Kyazumov	Mahmud	31		New rotation electron-diffraction methods and their applications	FIRST FLOOR	54	28 August, Wed.	MS16
Carlini	Lavinia	33		Protein Targeting to Glycogen (PTG), a validated target in Lafora disease	FIRST FLOOR	35	28 August, Wed.	MS10
Chrappan Soldavini	Benedetta	34		New ring-structured high pressure and temperature CaSiO3 polymorph and its stability field	FIRST FLOOR	89	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives

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Tragheim	Ben	35		Competition between G-type, C-type and CE-type orbital ordering modes in Na- and Ca-doped Hg-quadruple manganite perovskites	THIRD FLOOR	143	27 August, Tue.	MS29 - Structural characterization in Functional materials
Bataisai	Eustina	36		Gas sorption studies of mixed ligand metal-organic frameworks containing substituted diimide ligands	THIRD FLOOR	126	28 August, Wed.	MS30
Ali	Areesha	39	Vanessa Cascos; Stewart Clark; Manon Jones; Emma McCabe	Structure-composition relationships in layered perovskite-related materials	THIRD FLOOR	144	27 August, Tue.	MS29 - Structural characterization in Functional materials
Jacobs	Francois	41		In search of new interactions for rhenium metal-based pharmaceutical development.	FIRST FLOOR	36	28 August, Wed.	MS10
Petrovic	Marko	42	David McDonagh; David Waterman	Automating the 3DED/MicroED data processing at Diamond Light Source's Electron Bio-Imaging Centre	FIRST FLOOR	45	29 August, Thur.	MS22
Stanić	Petra	44		The role of multicentric pancake bond in 2D arrays of TCNQ radicals in crystals	FIRST FLOOR	80	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography
Molčanov	Krešimir	50		Extended motives of two-electron multicentre bonds (pancake bonds): from discrete dimers to 2D networks	FIRST FLOOR	81	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography
Cazzola	Davide	51	Davide Cazzola; Christoph Mueller-Dieckmann; Ehmke Pohl	Targeting the sphingolipid biosynthesis pathway of protozoan parasites as drug targets	FIRST FLOOR	24	27 August, Tue.	MS5 - Infectious and Neglected diseases
Butler	Abbey	52		Understanding the molecular basis of retinoid signalling	FIRST FLOOR	37	28 August, Wed.	MS10
van Staden	Christo	56		In "Au" Over Metallophilic Interactions	SECOND FLOOR	106	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Semjonova	Aina	57		Diversity and Similarity in Isonicotinamide Two-Component Phases with Alkyl Carboxylic Acids: Focus on Solvates	THIRD FLOOR	117	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Čerpakovska	Zane	58		Additive assisted mechanochemical control of caffeine:anthranilic acid co-crystal polymorphs	THIRD FLOOR	148	28 August, Wed.	MS40
Sanchez Rodríguez	Filomeno	59		Moorhen: interactive model building on the web	GROUND FLOOR	15	27 August, Tue.	MS4 - AI, software developments and Machine learning applied to MX and CryoEM
Gruene	Tim	62		Assignment of partial charges with 3D ED	FIRST FLOOR	82	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography
Friggeri	Laura	63	William Midgley; Ehmke Pohl; Bojana Popovic	Optimising GOLD pipelines for in silico PROTAC screening	FIRST FLOOR	38	28 August, Wed.	MS10
Deresz	Krystyna	64		Nitro-to-endo-nitrito isomerization in the solid state: unravelling light-induced mechanism of the process	FIRST FLOOR	57	29 August, Thur.	MS25
Posavec	Lidija	66		Ternary halogen-bonded cocrystal design using Ni(II) complex containing isothiocyanate ligands as halogen bond acceptor species	THIRD FLOOR	125	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Szymański	Bartosz	68		Shedding a new light on nitro compounds: NIR-emitting quadrupole-structured dyes	THIRD FLOOR	145	27 August, Tue.	MS29 - Structural characterization in Functional materials
Rybicka	Paulina Maria	69		local coordinate systems on local symmetry of atoms and atom types in the MATTS data bank	FIRST FLOOR	46	28 August, Wed.	MS11
Kumar	Anil	70		The charge density derived from electron diffraction on simulated data differs from that obtained from X-ray diffraction	FIRST FLOOR	43	27 August, Tue.	MS21 - Electron diffraction joining forces with quantum crystallography towards materials science applications
Cormack	Isabel	71	Ehmke Pohl; Bernd Striberny	Fantastic SSBs and where to find them	GROUND FLOOR	1	29 August, Thur.	MS01
Potempa	Kinga	72		Insights into role of non-covalent interactions in achieving pressure-induced linkage isomerism of nitrite ligand.	THIRD FLOOR	126	27 August, Tue.	MS31 - Noncovalent interactions in structure design

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Friedl	Sebastian	74		Pressure induced phase transition of [Ni(Tp*)(acac)(MeCN)]	FIRST FLOOR	98	28 August, Wed.	MS27
Satheasuweatha Marimuthu	Nirmala Devi	75		High-Pressure Structural Investigations of AuSn4 and its Potential Chemical Pressure Equivalent PtSn4	FIRST FLOOR	99	28 August, Wed.	MS27
Calora	Alessia	76	Matteo Calvaresi; Matteo Di Giosia; Giuseppe Falini; Silvia Fanti; Simona Fermari; José Gavira; Daniele Tedesco	BSA nanoparticles as innovative heterogeneous nucleants for protein crystallization	GROUND FLOOR	9	29 August, Thur.	MS08
Breen	Olivia	77		Synthesis of iron- and lithium- based oxalate compounds for use as cathode materials	THIRD FLOOR	146	27 August, Tue.	MS29 - Structural characterization in Functional materials
Wiseman	Amy	78		Metagenomic mining for cold adapted phage enzymes	FIRST FLOOR	34	27 August, Tue.	MS6 - Structural studies in Enzymology
Keene	Tony	79	Viktorija Mikaite	Rad(ical) Naphthalimide-Based Coordination Polymers	THIRD FLOOR	127	28 August, Wed.	MS30
Marchetti	Danilo	81	Moussa Diame Faye Diouf; Andrea Sala; Enrico Dalcanale; Alessandro Pedrini; Mauro Gemmi; Chiara Massera	Combined application of 3D electron diffraction analysis and mechanochemical synthesis for the investigation of novel nanocrystalline reticular materials	FIRST FLOOR	51	27 August, Tue.	MS20 - When can ED challenges XRD in small molecule crystallography?
Gabellini	Giuseppe	82		Alcohol Dehydrogenases as model enzymes to investigate nucleotide cofactor specificity	FIRST FLOOR	35	27 August, Tue.	MS6 - Structural studies in Enzymology
Rodić	Marko	83	Milan Nešić; Matic Lozinšek; Niko Radulović	Insight into α -iminoamidines: Hirshfeld atom refinement and evaluation of intermolecular interaction energies	FIRST FLOOR	47	28 August, Wed.	MS11
van Terwingen	Steven	84		Tailoring halogen bond donors for crystal engineering	THIRD FLOOR	118	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Hunter	Charlotte	85		EBNA1 PROTACS	FIRST FLOOR	39	28 August, Wed.	MS10
Gauffre	Pierre	86		Crystallographic structure of whole nsp14 from SARS-CoV-2 stabilised by a nanobody	FIRST FLOOR	36	27 August, Tue.	MS6 - Structural studies in Enzymology
Vijayakumar Syamala	Vishnu	87		Metallophilicity-assisted piezochromism in a Rh(I) complex: structural, energetic, electronic and spectroscopic investigations under pressure	FIRST FLOOR	100	28 August, Wed.	MS27
Ernst	Michelle	88		From capture to catalysis: Insights from atomistic simulations into MOF and COF host-guest interactions and guest dynamics	FIRST FLOOR	48	28 August, Wed.	MS11
Gatto	Claudia Cristina	89		Structural Design, Hirshfeld Analysis And Noncovalent Interactions Of Newly Synthesized Ni(II) Complex With A Dithiocarbazate Ligand	THIRD FLOOR	127	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Molčanov	Lidija	90	Krešimir Molčanov; Marijana Jurić; Luka Pavić	Charge transfer causes bulk conductivity through π -hole interactions	THIRD FLOOR	128	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Edkins	Katharina	91		Exploring co-crystallisation as a technique for taste-masking of nevirapine	THIRD FLOOR	119	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Selsabil Yeddiou	Belkis	92		Synthesis, crystal structure, Hirshfeld surface analysis and framework Energy study of a new Ni-Coordination complex with 1,10-phenanthroline	THIRD FLOOR	129	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Alberto	Roger	93	Roger Alberto; Vladimir Azov; Alice Brink; Dumisani Kama; Andreas Roodt	Exploring Novel Organometallic Compounds: Bridging Catalysis and Medicine through Crystallographic Insights	FIRST FLOOR	63	27 August, Tue.	MS33 - Correlate molecular structure with materials properties
Cagossi	Giorgio	94	Andrea Daolio	A novel family of hexanuclear macromolecular complexes obtained under ball-milling conditions	THIRD FLOOR	147	27 August, Tue.	MS29 - Structural characterization in Functional materials
Mokolokolo	Pennie	95		Rhodium(I) Carbonyl Complexes as Model Nano-Wired Assemblies	FIRST FLOOR	64	27 August, Tue.	MS33 - Correlate molecular structure with materials properties
DeBorggraeve	Wim	98	Joachim Demaerel; Eral Ismalaj; Bingyu Li; Kexin Su; Luc VanMeervelt; Steven Verhelst	Ex situ Generation of Thiazyl Trifluoride (NSF3) as a Gaseous SuFEx Hub	FIRST FLOOR	40	28 August, Wed.	MS10
Byun	Sujeong	100	Changkon Park; Jeong-Yong Suh; Claus-Peter Witte; Sangkee Rhee	Structure and allosteric regulation of the inosine 5'-monophosphate-specific phosphatase from <i>Saccharomyces cerevisiae</i>	FIRST FLOOR	37	27 August, Tue.	MS6 - Structural studies in Enzymology

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Thompson	Sam	101		Chiral substitutions for promoting polar materials discovery	THIRD FLOOR	148	27 August, Tue.	MS29 - Structural characterization in Functional materials
Du	Chao-Hung	102		Study of the electronic ordering in quantum materials of RbV3Sb5 and Ir2In8Se	FIRST FLOOR	35	29 August, Thur.	MS14
Pong	Way-Faung	103		Coupling between spin and lattice in an XY-like spin-glass (Ni0.40Mn0.60)TiO3	FIRST FLOOR	83	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography
Haozhe Liu	Arthur	104		Phase diagram determination at high-pressure and low-temperature conditions	FIRST FLOOR	101	28 August, Wed.	MS27
Ganguly	Sudakshina	107		AlphaFold Database and its impact on the crystallographic world	FIRST FLOOR	41	28 August, Wed.	MS10
Fang	Xue	109	Weiwei Cao; Pierre-Loup Savary; Victor Castaing; Ana Becerro; Cécile Genevois; Emmanuel Veron; Didier Zanghi; Matthew Dyer; Alessio Zandonà; Pierre Florian; Franck Fayon; Mathieu Allix; Michael Pitcher	Synthesis and structure of highly non-stoichiometric garnets RE3+xAl5-xO12 (0 < x < 0.6)	THIRD FLOOR	149	27 August, Tue.	MS29 - Structural characterization in Functional materials
Suryawanshi	Abhishek	111		Multiple high-resolution structures providing the insights of glucose tolerance in GH1 family β -glucosidases	FIRST FLOOR	38	27 August, Tue.	MS6 - Structural studies in Enzymology
Gatta	G. Diego	112		Structural evolution and pressure-driven phase transitions in hydrated borates	FIRST FLOOR	90	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Luhong-Wang Liu	Lisa	113		Pressure induced transitions in two types of engineering oxides	FIRST FLOOR	102	28 August, Wed.	MS27
Bogdanović	Milica	115		Pd(II) and Pt(II) complexes with N-benzylphenotiazine – Hirshfeld atom refinement and intermolecular interaction energies	FIRST FLOOR	49	28 August, Wed.	MS11
Benkanoun	Aouaouche	116		Structural description and thermal analysis of a new diphenate 1D coordination polymer	THIRD FLOOR	150	27 August, Tue.	MS29 - Structural characterization in Functional materials
Mauri	Anna	119		Unveiling the crystallochemistry of a soft covalent organic framework during benzene and cyclohexane adsorption by in situ powder X-ray diffraction	THIRD FLOOR	128	28 August, Wed.	MS30
Hans	Philipp	120	Gonca Dardeniz; Abdellatif Saadaldin; Latif Khan; Neva Stucchi; Giulia Franceschin; Samah Al Khasoneh; Gianluca Iori	Enhanced Characterization of Ancient Glasses through Advanced Tomographic Techniques @ SESAME Synchrotron	THIRD FLOOR	118	29 August, Thur.	MS36
Théron	Coline	124		X-ray powder diffraction: a hub in the integrative study of the schematic Holocene rock art	THIRD FLOOR	119	29 August, Thur.	MS36
Setshedi	Itumeleng	125		Supramolecular synthesis, crystallization, and co-crystallization of combination drugs for the inhibition of mycobacteria species	FIRST FLOOR	25	27 August, Tue.	MS5 - Infectious and Neglected diseases
Smith	Mark	126		The influence of reaction conditions on co-crystals of isoniazid derivatives	THIRD FLOOR	120	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Sacharczuk	Natalia	127	Anna Olejniczak; Maciej Bujak; Marcin Podsiadło	Molecular aggregations in crystals of butene isomers determined at high-pressure	FIRST FLOOR	103	28 August, Wed.	MS27
Maly	Martin	128		Work with serial crystallography data from CrystFEL and xia2.sx in CCP4 suite	GROUND FLOOR	7	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
Szymon Sobczak		130	Szymon Sobczak	Piezosolvatochromic insights into solvent-solute interactions	THIRD FLOOR	130	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Jarzemska	Katarzyna	131		Nanosecond-lived excimer observation in a rhodium(I) crystalline complex via time-resolved Laue diffraction	FIRST FLOOR	65	27 August, Tue.	MS33 - Correlate molecular structure with materials properties
Simbrunner	Josef	132		Searching for new polymorphs by epitaxial growth	THIRD FLOOR	149	28 August, Wed.	MS40
Zolotarev	Pavel	133		A tool for the analysis of the bond strength anisotropy and search for the low-periodic substructures in crystalline solids	FIRST FLOOR	46	29 August, Thur.	MS22

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Keil	Eleanor	135		Understanding Carbon Dioxide Uptake in ZIFs Via In-Situ Single Crystal Diffraction	FIRST FLOOR	58	29 August, Thur.	MS25
Sitshwele	Nazo	137		Influencing the reaction pathway in solid-state Diels-Alder cycloaddition using a vinyl substituent	GROUND FLOOR	8	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
Rouag	Raounek	140		Synthesis, crystal structure, biological properties and theoretical calculations of 2-(2-aminophenyl)-1H-benzimidazol-3-ium dichloride	THIRD FLOOR	151	27 August, Tue.	MS29 - Structural characterization in Functional materials
Benzitouni	Ines	141		Investigations of the biological activity of new sulfanilamide derivative: single crystal X-ray diffraction analysis, DFT computational, in-silico ADME and molecular docking studies.	THIRD FLOOR	152	27 August, Tue.	MS29 - Structural characterization in Functional materials
Bogdanovic	Milica	142	Marijana Kostic; Vukadin Leovac; Mirjana Radanovic; Ljiljana Vojinovic Jesic	Synthesis and crystal structure analysis of a Ni(II) complex with Schiff base 2,6-diacetylpyridine-adamantane-1-carbohydrazide	THIRD FLOOR	153	27 August, Tue.	MS29 - Structural characterization in Functional materials
Montebault	Clément	145		Degradation processes of colored papyri from Ancient Egypt	THIRD FLOOR	120	29 August, Thur.	MS36
Fonjallaz	Alexis	146		Parameter optimization for serial diffraction data analysis	FIRST FLOOR	47	29 August, Thur.	MS22
Batmanghelich	Shiva	148	Andrzej Katrusiak; Jakub Kaczkowski; Iwona Plowas-Korus	Resorcinol polymorphism: the lattice energy and conformers	SECOND FLOOR	104	28 August, Wed.	MS27
Kurlin	Vitaliy	150	Daniel Widdowson	Ultra-fast detection of (near-)duplicate structures across major crystal databases	FIRST FLOOR	48	29 August, Thur.	MS22
Sudol	Abigail	151		Extensive substrate recognition by streptococcal antibody-degrading enzymes	GROUND FLOOR	2	27 August, Tue.	MS02 - Hot structures
Marshall	George	152		Order-disorder control in functional oxides	THIRD FLOOR	154	27 August, Tue.	MS29 - Structural characterization in Functional materials
Curtis	Esther	153		Anisotropy of Oxide Ion Conductors	THIRD FLOOR	107	27 August, Tue.	MS28 - Structural characterization of Energy Harvesting and Conversion Materials
Stubbs	Jack	154		Droplet microfluidics for uniform microcrystallization and rapid mixing	GROUND FLOOR	9	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
Ratajczyk	Paulina	156	Michał Andrzejewski; Andrzej Katrusiak; Lucia Maini; Marianna Marchini; Francesco Marin; Szymon Sobczak	Pressure- and temperature-driven polymorphism in PDI-C6	SECOND FLOOR	105	28 August, Wed.	MS27
Privitera	Mario	157		Insight into structure and function of a Klebsiella phage capsular depolymerase: from a serendipitous finding to the design of active mini-enzymes against K. pneumoniae	FIRST FLOOR	42	28 August, Wed.	MS10
Alotaibi	Thamer	158		A systematic study of crystal size influence on Crystal Sponge experiment outcomes	THIRD FLOOR	129	28 August, Wed.	MS30
Sironi	Luca	159	Luca Sironi	Pre-nucleation clusters in liquid benzoic acid	THIRD FLOOR	131	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Macetti	Giovanni	160		Symmetry-constrained Monte Carlo for crystal structure prediction	THIRD FLOOR	121	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Kumar	Lavanya	161		Understanding the electronic structure of halogen bonding with heavy pnictogen acceptor atoms: Insights from charge density and DFT analysis	FIRST FLOOR	84	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography
Atamas	Anastasiia	163		Investigation of the molecular architecture of Candida auris ribosome	GROUND FLOOR	12	29 August, Thur.	MS09
Urzhumtsev	Alexandre	164		Direct real-space determination of atomic parameters from inhomogeneous cryoEM and crystallographic maps	GROUND FLOOR	16	27 August, Tue.	MS4 - AI, software developments and Machine learning applied to MX and CryoEM
Yano	Naomine	165		Development of time-resolved structural analysis environment at SPring-8 BL41XU	GROUND FLOOR	10	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
Novelli	Giulia	167		Investigating Pharmaceutical Solid Forms at High Pressure	SECOND FLOOR	106	28 August, Wed.	MS27

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Coles	Simon J	170	Peter Horton	Hands-on, challenge-based teaching in crystallography undergraduate practicals	THIRD FLOOR	135	27 August, Tue.	MS41 - Approaches and tools for learning crystallography efficiently and avoiding misconceptions
Losus	Renny Louis Anto Maria	175		Conformational diversity of tetra-O-ethyl-p-tert-butylcalix[4]arene and its molecular dynamics in the single-crystal unity	THIRD FLOOR	122	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Nemčovičová	Ivana	178		Small glycomimetic serves as antagonist to viral glycoprotein HCMV UL141 to inhibit the TRAIL death receptor binding	FIRST FLOOR	43	28 August, Wed.	MS10
Kaszubowski	Oskar	180		Combining SC-XRD, micro-PXRD and 3D ED in the structural description of dehydration of nucleotides and nucleotide-based drug crystals	FIRST FLOOR	52	27 August, Tue.	MS20 - When can ED challenges XRD in small molecule crystallography?
Töbrens	Daniel M.	181		Deep insights into energy materials utilizing anomalous X-ray diffraction	THIRD FLOOR	108	27 August, Tue.	MS28 - Structural characterization of Energy Harvesting and Conversion Materials
Woinska	Magdalena	182		Hirshfeld atom refinement for polymeric structures: MOFs and COFs	FIRST FLOOR	50	28 August, Wed.	MS11
Danylyuk	Oksana	183	Oksana Danylyuk	Host-guest interactions guide pentamidine folding inside and outside the cavities of macrocyclic hosts	THIRD FLOOR	132	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Ratcliff	William	186	Satvik Lolla; Haotong Liang; Aaron Kusne; Ichiro Takeuchi	Semi and self supervised approaches to space group and Bravais lattice determination	FIRST FLOOR	49	29 August, Thur.	MS22
Ceborska	Magdalena	191		3,4-disubstituted benzoic acids as cofomers in the salts and cocrystals of pyrimethamine	THIRD FLOOR	123	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Gurung	Kshitij	192	Klemen Motaln; Matic Belak Vivod	Solving ambiguities: redetermining the crystal structures of rare Ag(II) compound using 3DED	FIRST FLOOR	53	27 August, Tue.	MS20 - When can ED challenges XRD in small molecule crystallography?
Grabowsky	Simon	194		The untold story of the world's most common crystal structure	FIRST FLOOR	85	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography
Longcake	Alexandra	195		Crystallising natural products via high-throughput nanodroplet crystallisation protocols.	GROUND FLOOR	10	29 August, Thur.	MS08
Castiglione	Franca	196	Stefano Elli; Antonino Famulari; Javier Marti Rujas; Alessandro Zanotti	Molecular recognition of aromatics in spherical nanocages	THIRD FLOOR	130	28 August, Wed.	MS30
Kaźmierczak	Michał	199		What we have learned about negative linear compressibility studying cocrystal of 1,2-bis(4-pyridyl)ethane and fumaric acid	THIRD FLOOR	107	28 August, Wed.	MS27
Kkrarcha	Hadda	200		Lattice constants prediction and thermochemistry of hexahalometallate A ₂ MX ₆	THIRD FLOOR	155	27 August, Tue.	MS29 - Structural characterization in Functional materials
Folkers	Laura	203		Open the black box with X-Area's intuitive, interactive, and colourful data quality assessment graphics	THIRD FLOOR	128	29 August, Thur.	MS39
Folkers	Laura	204		What does CO ₂ look like? - Explaining Crystallography to elementary school kids with the "Maus" - one of Germany's longest running science TV shows for kids	THIRD FLOOR	136	27 August, Tue.	MS41 - Approaches and tools for learning crystallography efficiently and avoiding misconceptions
Pietrzak	Anna	205		Unraveling the mysteries of intramolecular hydrogen bonding defined by the phosphoryl group	FIRST FLOOR	92	29 August, Thur.	MS31
Brown	Stephen	206		Photoinitiated Single-Crystal to Single-Crystal Redox Transformations of Titanium-Oxo Clusters	FIRST FLOOR	81	28 August, Wed.	MS19
Kravets	Kateryna	208		Diversity of the host-guest crystalline assemblies of p-sulfonatocalix[n]arenes with benzamidines	FIRST FLOOR	93	29 August, Thur.	MS31
Burian	Max	210	Tilman Donath; Sascha Grimm; Sofia Trampari	PILATUS4 Hybrid Photon Counting Detectors for Efficient and Fast X-ray Diffraction	FIRST FLOOR	92	28 August, Wed.	MS24
Irmer	Erhard	211		Crystal Structure Analysis in School	THIRD FLOOR	137	27 August, Tue.	MS41 - Approaches and tools for learning crystallography efficiently and avoiding misconceptions

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Kubicki	Maciej	215		Experimental electron density distribution in cocrystals of theophylline and pyromellitic acid	THIRD FLOOR	136	28 August, Wed.	MS32
Garcia-Granda	Santiago	216		Pigments based in M ₂ SiO ₄ (M = Ni, Co) olivine solid solutions from SiO ₂ – rich compositions	FIRST FLOOR	91	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Mugnaioli	Enrico	217		A combination of X-ray and electron crystallographic methods for understanding the origin of sector-zoning birefringent garnets with almandine-grossular composition	FIRST FLOOR	82	28 August, Wed.	MS19
Grześkiewicz	Anita	219		Solid-to-solid phase transitions in two isostructural Bi(III) complexes and their solid solution.	THIRD FLOOR	150	28 August, Wed.	MS40
Golz	Christopher	220	Anna Krawczuk	Spironolactone Polymorphism: Do New Methods Yield New Insights?	THIRD FLOOR	151	28 August, Wed.	MS40
De Felice	Sofia	221		Structural and functional characterization of hyper-stable human serum albumin variants	FIRST FLOOR	24	29 August, Thur.	MS10
McDonagh	David	222		Predicting Protein Crystal Solvent Content with Machine Learning	FIRST FLOOR	50	29 August, Thur.	MS22
Du	Chao-Hung	223		Study of the electronic ordering in quantum materials of RbV ₃ Sb ₅ and Ir ₂ In ₈ Se	THIRD FLOOR	110	28 August, Wed.	MS29
Todorovic	Nikolina	225		Structure-based IgE-epitope investigation of the major cat allergen Fel d 4	FIRST FLOOR	26	27 August, Tue.	MS5 - Infectious and Neglected diseases
Moszczyńska	Ida	226		Competition between CH $\cdots\pi$ and CH \cdots M contacts in metallocenes structures	THIRD FLOOR	108	28 August, Wed.	MS27
Książek	Maria	227		Slow Thermally-Induced Spin Crossover in the Two-Dimensional Network [Fe(bbtr) ₃](BF ₄) ₂	THIRD FLOOR	109	28 August, Wed.	MS27
Gasser	Fabian	228		On the Lorentz correction for grazing incidence X-ray diffraction	SECOND FLOOR	105	29 August, Thur.	MS38
Kusz	Joachim	229		X-ray diffraction study of bis(tetrazolyl)alkane-based Fe(II) coordination polymers	THIRD FLOOR	111	28 August, Wed.	MS29
Suescun	Leopoldo	230		The search for the 4th stable polymorph of Lapachol	THIRD FLOOR	152	28 August, Wed.	MS40
Marek	Martin	231		Structural basis for NanoLuc luciferase action	GROUND FLOOR	3	27 August, Tue.	MS02 - Hot structures
Fando	Maria	233		Demystifying CCP4 Cloud concepts: safeguarding structure determination through data structure and automation	THIRD FLOOR	129	29 August, Thur.	MS39
Miloš	Sofija	235		Crystallography of the pressure-induced structural phase transitions in K ₂ Ca(CO ₃) ₂ and K ₂ Ca ₂ (CO ₃) ₃ carbonates	FIRST FLOOR	92	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Andreeva	Elena A.	236		Discovery of a novel iron-copper-sulfur cluster in a glucose-methanol-choline (GMC) oxidoreductase	FIRST FLOOR	39	27 August, Tue.	MS6 - Structural studies in Enzymology
Rainer	Daniel N.	237		Complementing XRD at the national level – 3DED and the UK National Electron Diffraction Facility (NEDF)	FIRST FLOOR	54	27 August, Tue.	MS20 - When can ED challenges XRD in small molecule crystallography?
de Sanctis	Daniele	238		Serial Microsecond Crystallography at ESRF-EBS	GROUND FLOOR	11	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
Chernyshov	Dmitry	239		Effect of X-ray radiation on structure and properties of molecular crystals: from damage to a fine tuning	FIRST FLOOR	66	27 August, Tue.	MS33 - Correlate molecular structure with materials properties

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Lazzari	Rémi	241		Surface and epitaxial stresses in supported metallic nanoparticles: transition from monolayer-thick 2D to 3D strained Ag nano-clusters on Al ₂ O ₃ (0001)	FIRST FLOOR	59	29 August, Thur.	MS25
Kapetanaki	Sofia	242		Study of the conformational dynamics of a bacterial photoactivated adenylate cyclase	GROUND FLOOR	12	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
Suh	Jeong-Yong	244		Structure-based design and optimization of fungal lipases to improve substrate binding and enzyme activity	FIRST FLOOR	40	27 August, Tue.	MS6 - Structural studies in Enzymology
Miletich	Ronald	245		Disordered rhombohedral K ₂ Ca ₂ (CO ₃) ₃ : a supposedly transient state within an ambiguous transformation route on decompression	FIRST FLOOR	93	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Patil	Sanket	246	Parijat Das; Dilip Badgujar; Prasenjit Bhaumik	Structural and functional analysis of a pore forming toxin from Streptococcus mitis	GROUND FLOOR	13	29 August, Thur.	MS09
Engel	Katja	247	Thomas Schleid	Rb ₄ [As ₂ S ₁₀]: A Rubidium Polythioarsenate(V) with an Unusual Discrete [S ₃ As ₅ (S ₂) ₂ As ₃] ⁴⁻ Anion	THIRD FLOOR	112	28 August, Wed.	MS29
Yusenko	Kirill	248		Crystal Chemistry of Octahedral Rhodium(III) Chloroamines	FIRST FLOOR	94	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Hu	Junyi	249		A six-membered ring molecular sieve achieved by 3D-3D topotactic transformation	THIRD FLOOR	131	28 August, Wed.	MS30
Weigel	Tina	250		Optimizing in Situ and Operando Experiments: Customized Sample Chamber with Heavy Load Goniometer	FIRST FLOOR	60	29 August, Thur.	MS25
Edwards	Matthew	251	Mark Senn	Restoring superconductivity in hole-doped Pr ₂ CuO ₄ via high-pressure phase transitions	THIRD FLOOR	113	28 August, Wed.	MS29
Naumkina	Yelizaveta	252		Characterization of Apremilast – halogen benzoic acids cocrystals	THIRD FLOOR	137	28 August, Wed.	MS32
Gilski	Mirosław	255		Unusual helical crystal packing of potassium-independent L-asparaginase from Phaseolus vulgaris	GROUND FLOOR	14	29 August, Thur.	MS09
Bistrović	Andrea	256	Silvana Raić-Malić; Mario Cetina	Structures and biological properties of mono- and bis-pseudopurines	FIRST FLOOR	67	27 August, Tue.	MS33 - Correlate molecular structure with materials properties
Malinska	Maura	258		Decoding Amino Acid@Cucurbit[7]uril through X-ray diffraction: Balancing Hydrophobicity and Ion-Dipole Interactions	FIRST FLOOR	94	29 August, Thur.	MS31
Hakala	B. Viliam	260	Sophia Kurig; Nicolas Walte; Karen Friese; Andrzej Grzechnik	Phase stability of V6O13 and synthesis of defect mixed-valence V _{0.92} O ₂ rutile at high pressures and temperatures	FIRST FLOOR	95	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Ors	Taylan	261	Irena Déroche; Jean-Louis Paillaud	Localization of Na ⁺ cations within nanosize ECR-1 using a 3D ED method	FIRST FLOOR	83	28 August, Wed.	MS19
Arletti	Rossella	266	Riccardo Fantini; Michael Fischer; Monica Argenziano; Roberta Cavalli; Lorenzo Mino	Enhanced Photostability and Efficacy of Hybrid Zeolite-Encapsulated UV Filters for Sunscreen Applications	THIRD FLOOR	114	28 August, Wed.	MS29
Bortel	Tyler	270	Peter Moeck	Detecting and Correcting Systematic STM Imaging Errors: Plane Symmetry of Graphite Calibration Samples	FIRST FLOOR	84	28 August, Wed.	MS19
Dadivanyan	Natalia	272	Lei Ding; Gwilherm Nénert; Maria Orlova	Crystallization of molecular glass: from amorphous state to new polymorphic forms in the API sodium naproxen	THIRD FLOOR	153	28 August, Wed.	MS40
Gorelik	Tatiana E.	273	Martin U. Schmidt	Stacking-disordered structure of Pigment Orange 13 (C ₃₂ H ₂₄ Cl ₂ N ₈ O ₂) from electron diffraction	FIRST FLOOR	29	28 August, Wed.	MS35
Le Garff	Paul	274		Supramolecular isomerism in coordination polymers of Cd(II) with an imidazole based dipodal ligand	THIRD FLOOR	138	28 August, Wed.	MS32
Pompidor	Guillaume	275		High throughput fragment screening at the beamline P11 at PETRA III	FIRST FLOOR	25	29 August, Thur.	MS10
Richert	Clemens	276		Second Generation Chaperones Support Cocrystallization of Long Flexible Chain Molecules	THIRD FLOOR	139	28 August, Wed.	MS32
Dohnálek	Jan	279	Barbora Brezovská; Hana Šanderová; Alena Křenková; Martin Hubálek; Mária Trundová; Kristýna	A novel mechanism of bacterial transcription initiation under HelD-mediated protection	GROUND FLOOR	2	29 August, Thur.	MS01

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Uribe Rincon	Carla Margarita	281		Structural and spectroscopic characterisation of schafarzikite-type PbSbMO ₄ (M = Cr, Fe, Mn)	FIRST FLOOR	96	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Kost	Niklas	283		Oxidation state of ultrasmall dodecylamine-coated palladium nanoparticles probed by X-ray techniques	THIRD FLOOR	115	28 August, Wed.	MS29
Kraut	Daniel	284		Polar amalgams: structure-property relations in bad metals	FIRST FLOOR	97	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Banerjee	Arpan	285		Biochemical and structural insights on pH-dependent cooperativity of glutamate dehydrogenase in <i>Saccharomyces cerevisiae</i>	FIRST FLOOR	41	27 August, Tue.	MS6 - Structural studies in Enzymology
Gruene	Tim	286	Jeroen Anton van Bokhoven	Direct quantification of Aluminum content in zeolites by Three-Dimensional Electron Diffraction	FIRST FLOOR	55	28 August, Wed.	MS16
Karlsen	Martin Aaskov	287		Digging deeper into the irreversible disordering of nanocrystalline TiO ₂ -rutile electrodes	FIRST FLOOR	30	28 August, Wed.	MS35
Etter	Martin	288		The Powder Diffraction and Total Scattering Beamline P02.1 at PETRA III, DESY	FIRST FLOOR	93	28 August, Wed.	MS24
Leubner	Nathan	289		In-situ characterization of the epitaxial growth of BaTiO ₃ thin films by pulsed laser deposition using synchrotron radiation	FIRST FLOOR	61	29 August, Thur.	MS25
Moroni	Marco	290		Rationalizing the chiroptical behaviour of chiral hybrid metal halides: the role of composition and crystal structure	THIRD FLOOR	116	28 August, Wed.	MS29
Ganesh	Bera	291		Structural Stability and Adsorption Behaviour of CO ₂ -Loaded Pure Silica CHA Zeolite under High Pressure conditions	FIRST FLOOR	80	29 August, Thur.	MS27
Ouali	Naima	292		Residual stresses determination and analysis in dissimilar rotary friction joints using X-ray diffraction method	THIRD FLOOR	117	28 August, Wed.	MS29
Fahl	Benjamin	295		An all-order phonon approach to thermal diffuse scattering	FIRST FLOOR	31	28 August, Wed.	MS35
Bjelcic	Monika	296		Introducing MicroMAX: Advanced Beamline for Serial Crystallography and Time-Resolved Studies	GROUND FLOOR	13	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
Gemmrich Hernández	Laura	297	Ute Kolb	Multi-method study of calcium-aluminate cement hydration and its crystal structures	FIRST FLOOR	76	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Sutula	Szymon	298		Too small for XRD but perfectly sized for ED	FIRST FLOOR	55	27 August, Tue.	MS20 - When can ED challenges XRD in small molecule crystallography?
Bombicz	Petra	299		Noncovalent interactions – an obscure aspect of the definition of isostructurality	FIRST FLOOR	95	29 August, Thur.	MS31
Suwinska	Kinga	302		Macrocyclic molecules as potential drugs carriers	FIRST FLOOR	96	29 August, Thur.	MS31
Dolomanov	Oleg	303		Olex2 and olex2.refine	FIRST FLOOR	56	28 August, Wed.	MS16
Dialpuri	Jordan	304		NucleoFind: A Deep-Learning Network for Interpreting Nucleic Acid Electron Density	GROUND FLOOR	3	29 August, Thur.	MS01
Krajnak	Matus	306	Gearóid Mangan	MerlinEM, the universal detector for 4D STEM and 3D ED	FIRST FLOOR	57	28 August, Wed.	MS16
Oeckler	Oliver	308	Paul Sicher	Fe-based skutterudite-like compounds	THIRD FLOOR	109	27 August, Tue.	MS28 - Structural characterization of Energy Harvesting and Conversion Materials
Andersen	Asser Sloth	311	Johansson; Thomas Kjeldsen; Peter Kurtzhals; Gerd Schluckebier	Application of structural insights in the molecular engineering of insulin for recombinant expression in yeast.	FIRST FLOOR	26	29 August, Thur.	MS10
Ellaway	Joseph	312		Advancing protein conformation analysis: A comprehensive clustering pipeline for the Protein Data Bank	FIRST FLOOR	51	29 August, Thur.	MS22
Tailleur	Elodie	313		A multipurpose diffractometer for advanced SC-XRD experiments under T, P, E and hv	FIRST FLOOR	62	29 August, Thur.	MS25

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Kamale	Chinmay	314		Structure-guided improvement of glucose tolerance and catalytic efficiency of β -glucosidase from <i>Clostridium thermocellum</i> for industrial bioethanol production	GROUND FLOOR	18	28 August, Wed.	MS06
Wong	Walter	316		Electron beam induced degradation of MAPbI ₃ revealed by low dose 3DED	THIRD FLOOR	110	27 August, Tue.	MS28 - Structural characterization of Energy Harvesting and Conversion Materials
Gjørup	Frederik	317		Real-time data analysis at the DanMAX materials science beamline	FIRST FLOOR	63	29 August, Thur.	MS25
Kleemiss	Florian	318		Machine guess of scattering factors - SALTED-NoSpherA2	FIRST FLOOR	51	28 August, Wed.	MS11
Wu	Shitao	319		The Development and Application of 3D ED method in Crystalline Porous Materials	THIRD FLOOR	132	28 August, Wed.	MS30
Virovets	Alexandr	320		Single-crystal XRD: Black box vs experienced crystallographer	THIRD FLOOR	130	29 August, Thur.	MS39
Nusser	Lukas	321		The first oxides with mercury in the formal oxidation state 0? A ₂ HgO (A = Cs, Rb) and Cs(Cs _{0.774} (7)K _{0.226} (7))HgO	FIRST FLOOR	77	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Madura	Izabela	322		Crystalline forms of vitamin B7 - an example of a crystal engineer's nightmare	THIRD FLOOR	140	28 August, Wed.	MS32
May	Nóra	324		Solid and solution state structures of Cu(II) – macrochelates developed for theranostic purposes	THIRD FLOOR	118	28 August, Wed.	MS29
Toms	Tom	325		Incommensurate displacive and occupational modulation in the structures of [FeCr _{1-x} (urea) ₆](NO ₃) ₃ (x = [0, 1]) complexes	FIRST FLOOR	36	29 August, Thur.	MS14
Liu	Jie	326		Investigation of A Novel Organocobalt Complex of B12 Model Catalyst	THIRD FLOOR	119	28 August, Wed.	MS29
Ebel	Ben	327		First implementation of tight-binding methods (xtB) for quantum crystallographic refinement	THIRD FLOOR	131	29 August, Thur.	MS39
Brüx	Daniel	328	Florian Kleemiss	Creation and Analysis of a Single Crystal X-ray Diffraction Experiment Benchmark Database	FIRST FLOOR	72	27 August, Tue.	MS37 - How to address questions, doubts and struggles of a young crystallographer
Zaytseva	Irina	329		Reactivity of the new caesium suboxometallate Cs ₇ MO ₄ (M = In, Sc)	FIRST FLOOR	78	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Schulze	Manuel	331		A previously unnoticed RE-TM-antimonide: CeFeSb ₃ .	THIRD FLOOR	120	28 August, Wed.	MS29
Hakanpää	Johanna	332		New access model at PETRA III & future PETRA IV beamline at DESY	FIRST FLOOR	57	27 August, Tue.	MS23 - Future of light sources and XFEL
Pavlyuk	Nazar	333	Volodymyr Pavlyuk; Helmut Ehrenberg; Grygoriy Dmytriv	Crystal structure and hydrogenation properties of the Mg ₆ CoSn ternary compound	THIRD FLOOR	111	27 August, Tue.	MS28 - Structural characterization of Energy Harvesting and Conversion Materials
Freitag-Pohl	Stefanie	334		Protein-Ligand Interactions with the Dianthus Screening Platform	FIRST FLOOR	27	27 August, Tue.	MS5 - Infectious and Neglected diseases
Néner	Gwilherm	336		In-situ investigation of water harvesting by CAU-10-OH metal organic framework: a 2-steps process	THIRD FLOOR	133	28 August, Wed.	MS30
Garriga	Damià	340		Scientific opportunities for SSX in MX beamlines at ALBA	GROUND FLOOR	14	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
Otteny	Markus	342		From Laves to Zintl: All(Mg _{1-x} In _x) ₂ compounds (All=Ca, Sr, Ba)	FIRST FLOOR	79	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Gatta	G. Diego	343		(P,T)-behavior of an intermediate scapolite of unusual 14/m symmetry	FIRST FLOOR	45	27 August, Tue.	MS18 - Crystal-chemistry of minerals in the Universe: genesis, phase stability, and planetological implications
Elsegood	Mark R.J.	344		3D ED and Synchrotron Radiation SCXRD Combine to Solve a Drug Identification Puzzle	FIRST FLOOR	56	27 August, Tue.	MS20 - When can ED challenges XRD in small molecule crystallography?

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Gateshki	Milen	347	Thomas Dortmann; Thomas Degen; Mustapha Sadki; Nicholas Norberg; Gwilherm Nenert	The effect of sample displacement in X-ray powder diffraction measurements with laboratory diffractometers	FIRST FLOOR	94	28 August, Wed.	MS24
Balasingham	Jonathan	348	Vitaliy Kurlin; Viktor Zamaraev	Applications of isometry invariants on material property prediction	FIRST FLOOR	68	27 August, Tue.	MS33 - Correlate molecular structure with materials properties
Fuentes-Montero	Luis	350	David Waterman; Gwyndaf Evans	Dui2, the new graphical user interface for Dials	GROUND FLOOR	18	27 August, Tue.	MS4 - AI, software developments and Machine learning applied to MX and CryoEM
Bu	Kejun	352	Yang Ding; Hazohe Liu; Xujie Lü; Anna Moliterni; Takeshi Nakagawa; Jasminka Popović; Martina Vrankić	Structure-property behaviour of $(\text{N}(\text{C}_2\text{H}_5)_3)_3\text{FeBr}_4$ powder under high pressure	FIRST FLOOR	81	29 August, Thur.	MS27
Dejoie	Catherine	353		Correcting the axial divergence from high-resolution powder diffraction data	FIRST FLOOR	95	28 August, Wed.	MS24
Bauer	Melanie	354	Ute Kolb	Structure elucidation of two different materials with TADF properties using three-dimensional electron diffraction	THIRD FLOOR	121	28 August, Wed.	MS29
Oksanen	Esko	357		Neutron structure of <i>Leishmania mexicana</i> triosephosphate isomerase variant E97Q reveals a possible general acid	GROUND FLOOR	19	28 August, Wed.	MS06
Jones	Andrew	360		X-ray diffraction for battery analysis	FIRST FLOOR	64	29 August, Thur.	MS25
Hinuma	Yoyo	361		Finding the Bravais lattice of a "1/N" size supercell from error-containing lattice parameters	FIRST FLOOR	52	29 August, Thur.	MS22
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Morana	Marta	366	Arianna Minelli; Alexei Bosak; Luca Bindi; Giovanni Orazio Lepore	Temperature dependence of single-crystal diffuse scattering in cupropearceite, $[\text{Cu}_6\text{As}_2\text{S}_7][\text{Ag}_9\text{Cu}_4]$	FIRST FLOOR	67	28 August, Wed.	MS17
Carloni	Giacomo	369	Quentin Gaday	Structural insights into cell septation in <i>Mycobacterium tuberculosis</i>	GROUND FLOOR	4	27 August, Tue.	MS02 - Hot structures
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Krause	Lennard	371		SINCRYS – single-crystal materials science beamline at MAX IV	FIRST FLOOR	58	27 August, Tue.	MS23 - Future of light sources and XFEL
Palerma	Marta	372		Crystal structures of human histone deacetylase 8 in complex with novel hydroxamic acid inhibitors	FIRST FLOOR	27	29 August, Thur.	MS10
Dudek	Marta	373	Agata Jeziorna; Przemyslaw Nowak; Dineshchakravarthy Senthurpandi	Rich polymorphic landscape of binary systems of meloxicam with imidazole and pyrazole	THIRD FLOOR	154	28 August, Wed.	MS40
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Chen	Shih-Lun	380		Theoretical and Experimental Investigations of X-ray Back Diffraction at Grazing Incidence	FIRST FLOOR	59	27 August, Tue.	MS23 - Future of light sources and XFEL
Esrafilii	Leili	381	Christophe M.L. Vande Velde	Hydrogen bond donating MOFs - synthesis and structure	THIRD FLOOR	134	28 August, Wed.	MS30
Cianci	Michele	384		Unravelling the mechanism of lipid – enzyme interactions in the limbus region of lipases at atomic resolution	GROUND FLOOR	20	28 August, Wed.	MS06
Round	Adam	385		The SPB/SFX instrument at the European XFEL - capabilities and scientific use cases for room temperature dynamics.	GROUND FLOOR	1	28 August, Wed.	MS03
Jia	Xu	386	Chongting Ren; Luc VanMeervelt	Crystallographic insights into diverse water stability mechanisms of Zn-MOFs	THIRD FLOOR	135	28 August, Wed.	MS30

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Boullay	Philippe	390	Sara Passuti; Adrian David; Emmanuel GUILMEAU	Crystal structures at the nanoscale with Scanning Electron Diffraction Tomography	FIRST FLOOR	59	28 August, Wed.	MS16
Maloney	Andrew G. P.	393		Correlating particle informatics with surface wetting measurements	FIRST FLOOR	69	27 August, Tue.	MS33 - Correlate molecular structure with materials properties
Santucci	Marco	394		PyFast-ADT: python-driven 3DED data collection and automatic crystal tracking	FIRST FLOOR	60	28 August, Wed.	MS16
Park	SoHyun	395		Second-harmonic generation effect enhanced by Li+ substitution for Na+ in (Li _x Na _{6-x})Mo ₉ O ₃₀	THIRD FLOOR	122	28 August, Wed.	MS29
Cabaj	Małgorzata	397		Exploring the influence of imperfections on 3D electron diffraction intensities through multislice simulations	FIRST FLOOR	61	28 August, Wed.	MS16
Solokha	Pavlo	398		Long period stacking ordered (LPSO) Y-Ni-Mg phases studied by 3D electron diffraction	FIRST FLOOR	38	29 August, Thur.	MS14
Gladyshevskii	Roman	399	Svitlana Pukas	Quaternary compounds in R–T–Al–M systems	THIRD FLOOR	123	28 August, Wed.	MS29
Wehlander	Gabrielle	400		Exploring serial crystallography for capturing Michaelis complexes of a glucuronyl esterase involved in lignocellulose degradation	GROUND FLOOR	2	28 August, Wed.	MS03
Clough	Lewis	407		The high pressure behaviour of Nd(XeF ₂) ₃ (TaF ₆) ₃	FIRST FLOOR	82	29 August, Thur.	MS27
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Krysiak	Yaşar	409		High temperature electron diffraction on organic crystals: in situ crystal structure determination of Pigment Orange 34	GROUND FLOOR	18	29 August, Thur.	MS20
Ślepokura	Katarzyna	410		Structural description of dehydration and polymerization in cGMP crystals in light of the origins of life.	THIRD FLOOR	135	29 August, Thur.	MS40
Arhangelskis	Mihails	411	Sibananda Dash	Parameterization of an intermolecular forcefield for halogen bonded molecular crystals	FIRST FLOOR	98	29 August, Thur.	MS31
Schmitt	Yann	412		Challenging shortcomings in the field of 3D ED: a new cross-platform solution for various experimental set-ups	FIRST FLOOR	62	28 August, Wed.	MS16
Day	Maxwell	416		RamanCrystalHunter: a new program and database for processing, analysis, and identification of Raman spectra	FIRST FLOOR	47	27 August, Tue.	MS18 - Crystal-chemistry of minerals in the Universe: genesis, phase stability, and planetological implications
Bolton	Rachel	417	Robin Owen; Ivo Tews	SSX and SFX probe the cyanobacterial FutA iron binding protein by X-ray induced photoreduction and reveal a switch for Fe(II) / Fe(III) binding	GROUND FLOOR	3	28 August, Wed.	MS03
Radanović	Mirjana	420		Crystal structure of a copper(I) complex with the Schiff base of 2-(diphenylphosphino)benzaldehyde and aminoguanidine	THIRD FLOOR	125	28 August, Wed.	MS29
Schmidt	Ashley	423		Squeezing the most out of your high pressure data	FIRST FLOOR	83	29 August, Thur.	MS27
Khadiev	Azat	424	Dmitri Novikov; Madhenahalli Bhyrappa Sreedhara; Reshef Tenne	Particle- and Phase-selectivity with Micro and Macro X-ray beam at DESY P23 beamline: The Case of Ta_5S_{19} Nanotubes	FIRST FLOOR	85	28 August, Wed.	MS19
Henriques	Margarida	425		Incommensurate magnetic modulations of the 2D-layered Ho ₃ Co described by superspace symmetry	FIRST FLOOR	86	28 August, Wed.	MS19

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Alexander	Orbett	426		Metallo-organic chemistry of inert d6-low spin Rel-tricarbonyl synthon	FIRST FLOOR	70	27 August, Tue.	MS33 - Correlate molecular structure with materials properties
Merlini	Marco	427		The effect of iron on high-pressure behavior and phase transition in srebrodolskite-brownmillerite (CaFeO _{2.5} -CaAlO _{2.5})	FIRST FLOOR	48	27 August, Tue.	MS18 - Crystal-chemistry of minerals in the Universe: genesis, phase stability, and planetological implications
Tedesco	Consiglia	429		The peptoid's path to understand the role of CH ⁺ ···OC and CO ⁺ ···CO interactions in proteins	FIRST FLOOR	99	29 August, Thur.	MS31
Agarwal	Harshit	430		Charge density wave structural phase transition in SrAl ₂ Ga ₂	FIRST FLOOR	39	29 August, Thur.	MS14
Kohli	Varun	431		Tuning LLM models to predict protein's 3D structure	GROUND FLOOR	19	27 August, Tue.	MS4 - AI, software developments and Machine learning applied to MX and CryoEM
Sun	Yuh-Ju	434	Chen-Hsi Chu; Min-Guan Lin; Chwan-Deng Hsiao	Insights into the molecular mechanism of ParABS system in chromosome partition by HpParA and HpParB	GROUND FLOOR	6	29 August, Thur.	MS01
Ho	Feng-Hua	435		Structure Determinations and Phase Transition Study on New One-dimensional Fe(II) Coordination Polymers Using Tetrazole Derivatives	FIRST FLOOR	71	27 August, Tue.	MS33 - Correlate molecular structure with materials properties
Hsu	I-Jui	436		Characterization of phase transition behaviors of iron complexes based on pyridyl-tetrazole ligands	THIRD FLOOR	107	29 August, Thur.	MS33
Chandra	Mohit	439		Investigation of structural correlations at dielectric and magnetic ordering in Cr/Fe doped alpha-Mn ₂ O ₃	THIRD FLOOR	142	29 August, Thur.	MS29
Kremer	Marius	440		New developments in non-ambient X-ray diffraction instrumentation	FIRST FLOOR	96	28 August, Wed.	MS24
McPherson	James	441	James McPherson	Metal-organic frameworks with zero-valent metal nodes	GROUND FLOOR	19	29 August, Thur.	MS20
Kim	Hye-Yeon	442		Structural and biophysical characterization of antigen-antibody complexes	FIRST FLOOR	29	27 August, Tue.	MS5 - Infectious and Neglected diseases
Friedly	Alexandra	444		Surprising Formation of a [Bi ₆ O ₄ (OH) ₄] ⁶⁺ Cation in the Dodecahydro-closo-Dodecaborate Hydrate [Bi ₆ O ₄ (OH) ₄][B ₁₂ H ₁₂] ₃ · 10 H ₂ O	THIRD FLOOR	143	29 August, Thur.	MS29
Jurić	Marijana	446	Ana Lozančić; Sanja Burazer; Sanja Renka; Krešimir Molčanov; Lidija Androš Dubraja	Structural, conductive and precursor properties of heterometallic compounds containing alkylammonium cations	THIRD FLOOR	108	29 August, Thur.	MS33
Goetz	Emila	447	Krivovichev; Michael Czank; Marco Schowalter; Lukas Palatinus; Ira V. Rozhdersvenskaya; Viktor N. Yakovenchuk; Ute Kolb	Eveslogite – a highly complex nanotubular titanosilicate mineral solved by 3D ED	FIRST FLOOR	68	28 August, Wed.	MS17
Serrão	Guilherme	450		Quinolines as optimal Halogen-Bonding acceptors	FIRST FLOOR	100	29 August, Thur.	MS31
Tiwari	Bhaskar	451		Polymorphism of ribavirin at high pressure	THIRD FLOOR	136	29 August, Thur.	MS40
Orr	Christian	453		Spherical Crystals: Laser Shaping of Biological and Chemical Materials	FIRST FLOOR	60	27 August, Tue.	MS23 - Future of light sources and XFEL
Kovalevskiy	Oleg	454		The next generation of AlphaFold: accelerating structural biology research	GROUND FLOOR	20	27 August, Tue.	MS4 - AI, software developments and Machine learning applied to MX and CryoEM
Hulai	Natalia	455	Daniels; Matthew S. Dyer; Cara J. Hawkins; Bhupendra Mali; Jon A. Newnham; Hongjun Niu;	Navigation through high-dimensional chemical space: discovery of two Ba-Y silicates	FIRST FLOOR	69	28 August, Wed.	MS17
Del Giudice	Alessandra	456	Libero Gurrieri; Paolo Trost; Roberto Marotta; Francesca Sparla; Simona Fermani	Regulation pathway of photosynthetic glyceraldehyde 3-phosphate dehydrogenase	GROUND FLOOR	21	28 August, Wed.	MS06
Gesing	Thorsten M.	457		Determination of the average crystallite size and the crystallite size distribution: The envelope function approach EnvACS	FIRST FLOOR	70	28 August, Wed.	MS17

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Hari	Krishna	460		Biological piezoelectric materials as high-performance, eco-friendly structural health monitors	THIRD FLOOR	112	27 August, Tue.	MS28 - Structural characterization of Energy Harvesting and Conversion Materials
Elliott	Luc	461		Slice'N'Dice: Maximising the value of predicted models for structural biologists	FIRST FLOOR	53	29 August, Thur.	MS22
Biran	Ido	462	Alexei Bosak; Zuo-Guang Ye; Igor Levin; Semën Gorfman	Lattice match between coexisting cubic and tetragonal phases in PMN-PT at the phase transition	THIRD FLOOR	144	29 August, Thur.	MS29
Grybauskas	Algirdas	463		Method of extending rotamer libraries and its usage in protein active site studies	GROUND FLOOR	22	28 August, Wed.	MS06
Gašparíková	Dorota	465		Glucokinase and structure-based drug discovery	FIRST FLOOR	28	29 August, Thur.	MS10
Vypřitskaia	Angelina	466		Neural Network-Assisted Crystal Detection for Automated Electron Diffraction Data Collection	FIRST FLOOR	63	28 August, Wed.	MS16
Schleid	Thomas	467	Felix Christian Goerigk	Gd ₂ F[CO ₃][AsO ₃]: A Serendipitously Formed Gadolinium Fluoride Oxocarbonate Oxoarsenate(III)	FIRST FLOOR	71	28 August, Wed.	MS17
Locke	Ralf Jules Christian	468	Thomas Schleid	Closing Some Gaps of Knowledge: Single Crystals of Nd ₂ [Sb ₄ O ₈]Cl ₂	FIRST FLOOR	72	28 August, Wed.	MS17
Locke	Ralf Jules Christian	469	Thomas Schleid	Pr ₃ OI[AsO ₃] ₂ : The First Oxide Iodide Oxoarsenate of the Rare-Earth Metals	FIRST FLOOR	73	28 August, Wed.	MS17
Lissner	Falk	470	Thomas Schleid; Kurt Walenta	The Trigonal Crystal Structure of Matildite-Type AgBiS ₂ Revisited	FIRST FLOOR	74	28 August, Wed.	MS17
Kedari	Ashwini	471	ASHWINI KEDARI	Structural perspective into rabies virus neutralization	FIRST FLOOR	30	27 August, Tue.	MS5 - Infectious and Neglected diseases
Rzepka	Przemyslaw	474		Determining Active Sites in Zeolite Structures Using Anomalous Diffraction at the Al K-edge	FIRST FLOOR	73	29 August, Thur.	MS30
Stürzer	Tobias	475		Masterful sample grilling starts here	FIRST FLOOR	75	28 August, Wed.	MS17
Clarke	Brendan	477		Applications of precession-assisted scanned nanobeam diffraction tomography to sample metrology over large ROIs	FIRST FLOOR	64	28 August, Wed.	MS16
Thompson	Paul	478		Diffraction (AXRD) Interleaved with X-ray Absorption Spectroscopy (XAS) Using a Scanning 2D Imaging Detector at the XMaS Beamline	FIRST FLOOR	97	28 August, Wed.	MS24
Crichton	Wilson	479		The EBS large volume press facility at the ESRF	FIRST FLOOR	84	29 August, Thur.	MS27
Lahey-Rudolph	Mia	480		Crystals in living insect cells: Of detection, serial diffraction and genuine co-factor discovery.	GROUND FLOOR	4	28 August, Wed.	MS03
Aghaei Hakkak	Rouzbeh	481		(CN ₅ H ₄) ₂ [B ₁₂ H ₁₂] · 2 H ₂ O: A Low-Carbon High-Energy Compound Based on 5-Aminotetrazolium and Dodecahydro-closo-Dodecaborate Ions	FIRST FLOOR	76	28 August, Wed.	MS17
Scatena	Rebecca	488		Hybrid improper ferroelectricity in columnar (Na ₃)MnMnTi ₄ O ₁₂	THIRD FLOOR	145	29 August, Thur.	MS29
Lampronti	Giulio Isacco	489		The scientific case for in-situ diffraction investigations of mechanochemical processes: recent developments and state of the art.	FIRST FLOOR	65	29 August, Thur.	MS25
Kurlin	Vitaliy	491		The Crystal Isometry Principle has made transparent the black boxes of structural databases	THIRD FLOOR	132	29 August, Thur.	MS39
Cesselli	Daniela	492	Marta S. Semrau; Paola Storici	ULK1 inhibition for autophagy deregulation recovery	FIRST FLOOR	29	29 August, Thur.	MS10

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Anosova	Olga	493	Vitaliy Kurlin	Richard Feynman's visual hint gave birth to a new area of continuous crystallography	SECOND FLOOR	106	29 August, Thur.	MS38
Gonen	Tamir	494	Jieye Lin; Johan Unge	Automated MicroED as a powerful powder diffraction tool for complex samples	GROUND FLOOR	20	29 August, Thur.	MS20
Sangster	Calum	495	Fabio Nudelman	Use of 3D-ED as a Tool for Studying Mechanism of Formation of Complex Materials	GROUND FLOOR	21	29 August, Thur.	MS20
Vaitkus	Antanas	496		Lost in translation – using CIF dictionaries for semantic data validation	THIRD FLOOR	125	29 August, Thur.	MS38
Merkys	Andrius	497		Quality control of the chemical information in the Crystallography Open Database	THIRD FLOOR	133	29 August, Thur.	MS39
Kingsbury	Christopher J.	499		Molecular symmetry and art: visualizing the near-symmetry of molecules in Piet Mondrian's De Stijl	FIRST FLOOR	99	27 August, Tue.	MS26 - Chirality: Meeting point of crystallography, chemistry and topology
Lin	Hong-Cheu	502		Elastomers Containing Innovatively Modified [c2] Daisy Chain Molecules with Promoted Stretchabilities and Toughnesses	THIRD FLOOR	146	29 August, Thur.	MS29
Braun	Maxime	503		Anti-magnetolectricity, a hidden order probed by Dynamical Magnetic Charges	FIRST FLOOR	87	28 August, Wed.	MS19
Gao	Yunyun	504		A Robust Beamstop Shadow Outlier Rejection: Combining Crystallographic Statistics with Modern Clustering Method	FIRST FLOOR	54	29 August, Thur.	MS22
Bramantya	Bramantya	505		Ab initio crystal structure prediction (CSP) of magnetic metal-organic frameworks (MOFs)	FIRST FLOOR	88	28 August, Wed.	MS19
Wang	Gang	507		Topological crystalline insulator candidate ErAs ₅ with hourglass fermion and magnetic-tuned topological phase transition	THIRD FLOOR	113	27 August, Tue.	MS28 - Structural characterization of Energy Harvesting and Conversion Materials
Krengel	Ute	508		New structural insights into bacterial colonization by <i>Vibrio cholerae</i>	GROUND FLOOR	10	28 August, Wed.	MS05
Heine	Andreas	509		Fragment-based inhibitor development to fight Shigellosis	GROUND FLOOR	11	28 August, Wed.	MS05
Saric	Lovro	512	Georgia Cametti; Ivica Zivkovic	Reinvestigation of the crystal structure and magnetic properties of M(VO) ₂ (PO ₄) ₂ ·4H ₂ O and Ni _{0.5} (VO) ₂ (PO ₄) ₂ ·1.5H ₂ O (M = Ni ²⁺ , Co ²⁺) compounds	FIRST FLOOR	77	28 August, Wed.	MS17
Hu	Chengdao	514	Cameron J. G. Wilson; Simon Parsons	Centring of Diamond Anvil Cells Using an Optical Sensor	FIRST FLOOR	85	29 August, Thur.	MS27
Francia	Nicholas	515		Comparison of crystal structure similarity algorithms and analysis of large sets of theoretically predicted structures	FIRST FLOOR	55	29 August, Thur.	MS22
Percoco	Rita Maria	516		Novel BioMOF@PAN Mixed Matrix Membranes as Highly Per-formant Adsorbing Materials for Multiple Heavy Metal Ions Removal	FIRST FLOOR	74	29 August, Thur.	MS30
Iqbal	Waseem	517		Efficient Nickel and Cobalt Recovery by Metal–Organic Framework based Mixed Matrix Membranes (MMM-MOFs)	FIRST FLOOR	75	29 August, Thur.	MS30
Ward	Martin	518		Pushing Technique Boundaries to Probe Conformational Polymorphism	THIRD FLOOR	137	29 August, Thur.	MS40
Bereczki	Laura	520	Petra Bombicz; Sourav De; Gabriella Györík; Tamás Holczbauer; Nóra Veronika May; András Tompos; Zoltán Varga; András Wacha	Curious Chemist summer camp at the Research Centre for Natural Sciences in Hungary	THIRD FLOOR	138	27 August, Tue.	MS41 - Approaches and tools for learning crystallography efficiently and avoiding misconceptions
Adjimani	Joseph	521	Laszlo Fabian; Yaroslav Khimiyak	Balancing Act: Studying Stoichiometry in Hydroxybenzoic Acid-Cyclic Amide Cocrystals with X-Ray Diffraction and In-situ solid state NMR	THIRD FLOOR	141	28 August, Wed.	MS32
Rosa	Patrick	522		Molecular ceramics of spin crossover materials by Cool-SPS for barocaloric refrigeration	FIRST FLOOR	86	29 August, Thur.	MS27
Jandl	Christian	523	Benjamin A. Palmer; Laura Samperisi	Electron diffraction for direct structural determination of biogenic crystals	GROUND FLOOR	22	29 August, Thur.	MS20

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Weber	Thomas	527	Joohee Bang	Understanding complex order in thin film structures with the 3D-PDF method	FIRST FLOOR	44	27 August, Tue.	MS34 - Applications of 3D-PDF
Ward	Suzanna	531		A toolkit for young crystallographers in need of more learning resources	FIRST FLOOR	73	27 August, Tue.	MS37 - How to address questions, doubts and struggles of a young crystallographer
Tarantino	Serena Chiara	532		A crystallographic approach to the study of dinosaur eggshells of 70 Ma from Mexico	THIRD FLOOR	121	29 August, Thur.	MS36
Götz	Emilia	536		Exploring new features in sub-micron crystal structure analysis with the XtaLAB Synergy-ED	FIRST FLOOR	65	28 August, Wed.	MS16
Gladyshevskii	Roman	538	Yaroslav Tokaychuk	Crystal structures of the phases in the systems T5M3–T5M'3 (T = Ti, Zr, Hf; M = Al, Ga; M' = Si, Ge, Sn, Pb, Sb, Bi)	THIRD FLOOR	147	29 August, Thur.	MS29
Joseph	Boby	539		Hard X-ray Diffraction Beamlines at Elettra for Material Science : The Present and the Future	FIRST FLOOR	61	27 August, Tue.	MS23 - Future of light sources and XFEL
Lübben	Anna	545		Leveraging Deep Learning for smart sample alignment	GROUND FLOOR	21	27 August, Tue.	MS4 - AI, software developments and Machine learning applied to MX and CryoEM
Perles	Josefina	546		Mn(II) organo-inorganic salts as stimulus-responsive luminescent compounds	THIRD FLOOR	109	29 August, Thur.	MS33
Mazzeo	Paolo P.	547		On the Mechanism of Cocrystal Formation by Mechanochemical Reaction via Low Melting Eutectic: A Time-Resolved In Situ Monitoring Investigation	FIRST FLOOR	101	29 August, Thur.	MS31
Round	Ekaterina	551		Integrated sample preparation, characterization and delivery for room temperature serial crystallography at the European XFEL	GROUND FLOOR	5	28 August, Wed.	MS03
Psycharis	Vassilis	552		Structure relations of belite and alite polymorphs	FIRST FLOOR	78	28 August, Wed.	MS17
Gollé-Leidreiter	Philipp	554		The crystal structures of two Y2O3 and B2O3 containing pyroxenes	FIRST FLOOR	79	28 August, Wed.	MS17
Neels	Antonia	555		Complex nanoparticle systems in motion: a holistic analytical approach for dynamical studies in biological environments	FIRST FLOOR	66	29 August, Thur.	MS25
Borovina	Mladen	556	Ivan Kodrin; Mateja Pisačić; Matteo Zausnig; Marijana Đaković	Mechanoflexibility in crystalline coordination polymers: Correlating mechanical properties with structural prerequisites and consequences	THIRD FLOOR	110	29 August, Thur.	MS33
Strzalka	Radoslaw	558		The real space approach to the atomic structure of Tsai-type quasicrystal	FIRST FLOOR	40	29 August, Thur.	MS14
Wolny	Janusz	559		Quarter century of the statistical method in crystallography	FIRST FLOOR	41	29 August, Thur.	MS14
Qi	Ji	560		Correlation between structure and dynamic properties in SCO complex Fe(PM-BIA)2(NCS)2	THIRD FLOOR	148	29 August, Thur.	MS29
Pfanzagl	Vera	562		Myeloperoxidase dimerization in solution is mediated by interface glycans	GROUND FLOOR	23	28 August, Wed.	MS06
Kováts	Éva	563	Dávid Földes; Gábor Bortel; Sándor Pekker	A new chiral metal-organic framework with spiranes	FIRST FLOOR	76	29 August, Thur.	MS30
Karimova	Oxana	565		High temperature single crystal X-ray diffraction of Pd bismuthides	FIRST FLOOR	87	29 August, Thur.	MS27
Chintakindi	Hrushikesh	567	Lukas Palatinus	Analysing the frame scaling and orientation matrix in the presence of appreciable dynamic diffraction effects utilizing simulated 3D ED data	FIRST FLOOR	66	28 August, Wed.	MS16
Dranka	Maciej	568		Utilizing structural studies for developing a new concept of aqueous electrolytes based on lithium 4,5-dicyanoimidazole hydrates	THIRD FLOOR	111	29 August, Thur.	MS33
Vascon	Filippo	569	Matteo Bersani; Eleonora Gianquinto; Alice Legru; Federica Verdirosa; Laurent Gavara; Donatella Tondi; Francesca Spyrikis; Loretta Lazzarato; Jean-Francois Hernandez; Jean-Denis Docquier; Laura Cendron	X-ray crystallography deciphers the inhibition of thione-based compounds on NDM-1 b-lactamase	GROUND FLOOR	12	28 August, Wed.	MS05

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Hordiichuk	Oleh	570		Hybrid materials of metal halide nano-sized clusters orderly confined in single crystal metal-organic reticular materials	FIRST FLOOR	77	29 August, Thur.	MS30
Luneau	Dominique	571		Electron diffraction boosts research on molecule-based magnets	FIRST FLOOR	89	28 August, Wed.	MS19
Saridakis	Emmanuel	572		Protein thermodynamic properties, crystallisation, and the Hofmeister Series	GROUND FLOOR	11	29 August, Thur.	MS08
Ribaldone	Chiara	574		Combining Molecular Dynamics Simulations with Topological Analysis of the Bonding in Crystalline Systems	FIRST FLOOR	86	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography
Cholakova	Diana	575	Nikolai Denkov; Slavka Tcholakova	Polymorphism in triglyceride systems: in bulk and in emulsion droplets	THIRD FLOOR	138	29 August, Thur.	MS40
Kholina	Yevhenia	576	Arkadiy Simonov	Unconventional charge transfer transition in KCo[Fe] Prussian Blue Analogue	THIRD FLOOR	149	29 August, Thur.	MS29
Hikita	Masahide	578		Current status of microspectroscopic systems for the macromolecular crystallography beamline AR-NW12A at the Photon Factory	GROUND FLOOR	6	28 August, Wed.	MS03
Baisch	Ulrich	580		Ion-induced cocrystallisation and polymorph Screening	THIRD FLOOR	139	29 August, Thur.	MS40
Friese	Karen	581		Incommensurate structures and radiation damage in K2V3O8 and Rb2V3O8 mixed-valence vanadate fresnoites	FIRST FLOOR	42	29 August, Thur.	MS14
Rečko	Katarzyna	584	Marta Orzechowska; Maria Biernacka; Beata Kalska-Szostko	Magnetism of gallium cuboferrites	THIRD FLOOR	150	29 August, Thur.	MS29
De	Sourav	586		The effect of high pressure on the crystal structure of organocatalysts	FIRST FLOOR	88	29 August, Thur.	MS27
Dereze	Solomon	589	Juan Manuel Garcia-Ruiz; Patricia Gitari; Joy Kiano; Martin Mbugua; Fermin Otalora	The Africa Education Program for Training Kenyan High school Teachers on "Learning how Science works with crystals" and the First African Crystallization Contest in the Schools	THIRD FLOOR	139	27 August, Tue.	MS41 - Approaches and tools for learning crystallography efficiently and avoiding misconceptions
Grineva	Olga	590		Comparative analysis of the magnetic properties of organic compounds without metal atoms and their molecular and crystal structures	THIRD FLOOR	112	29 August, Thur.	MS33
Aguiar Suescun	Ivana	591	Emiliano García; Aylene Grenni; Noella Méndez; Florencia Menéndez; Federico Mesa; Maia Momburó; Ivana Núñez; Santiago Ploli; Carlos Rojas; Leopoldo	CNCC - Concurso Nacional de Crecimiento de Cristales de Uruguay: 10 years of a successful crystal growing competition for schoolchildren and more.	THIRD FLOOR	140	27 August, Tue.	MS41 - Approaches and tools for learning crystallography efficiently and avoiding misconceptions
Chinellato	Monica	592		Class IIa HDAC derived peptides elucidate the promiscuous binding to myocyte enhancer factor-2 in complex with DNA	FIRST FLOOR	30	29 August, Thur.	MS10
Parisi	Emmanuele	593		Controlling particle properties via crystal engineering: an example on quercetin hydrates, solvates and cocrystals.	THIRD FLOOR	142	28 August, Wed.	MS32
Heinemann	Udo	595	Qianqian Ming; Yvette Roske; Maria Rutkiewicz; Jianhui Wang	Structural and target DNA-binding studies of Grainyhead/CP2 transcription factors	GROUND FLOOR	7	29 August, Thur.	MS01
Krengel	Ute	597	Natalia Mojica	Structural basis for the differential toxicity of cholera toxin and heat-labile enterotoxin	GROUND FLOOR	13	28 August, Wed.	MS05
Uski	Ville	598	Ville Uski	Introducing the next major release of CCP4: What's new?	GROUND FLOOR	22	27 August, Tue.	MS4 - AI, software developments and Machine learning applied to MX and CryoEM
Schirò	Giorgio	601		Structural dynamics of a B12-dependent photoreceptor	GROUND FLOOR	7	28 August, Wed.	MS03
Lazarova	Hristina	606		Grace titanium silicate-1 for treatment of Crystal violet and Methylene blue by wastewater	FIRST FLOOR	78	29 August, Thur.	MS30
Pindelska	Edyta	607		New multicomponent systems of the anti-cancer drug erlotynib	THIRD FLOOR	143	28 August, Wed.	MS32
Raptoupoulou	Catherine	608		Chiral heterometallic Cu/Ln complexes from enantiopure Schiff base ligands	FIRST FLOOR	100	27 August, Tue.	MS26 - Chirality: Meeting point of crystallography, chemistry and topology

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Coles	Simon	612		Raw Data Letters - describing and publishing raw diffraction data in a FAIR way	THIRD FLOOR	126	29 August, Thur.	MS38
Catapano	Lucrezia	613		Enhancing structural refinement of macromolecules obtained from neutron crystallography	FIRST FLOOR	28	28 August, Wed.	MS06
Li	Zhao	617		In situ synchrotron-based grazing incidence X-ray diffraction study on the solid-liquid interface of graphene oxide	FIRST FLOOR	67	29 August, Thur.	MS25
Slawinski	Wojciech	618		BIG BOX modelling of Pair Distribution Function using RMCProfile7 program	FIRST FLOOR	32	28 August, Wed.	MS35
Kretić	Danijela	623	Aleksandra Đunović; Ivana Veljković; Dušan Veljković	How do non-covalent interactions affect the sensitivity of high-energy materials? Analysis of crystal structures of nitroaromatic molecules.	THIRD FLOOR	113	29 August, Thur.	MS33
Johansen	Morten	624		Structural effects from varying the Fe/Mn ratio in layered NaFeyMn1-yO2 for Na-ion batteries	FIRST FLOOR	68	29 August, Thur.	MS25
Crowley	Peter	625		Protein assembly and crystallization with synthetic macrocycles	THIRD FLOOR	144	28 August, Wed.	MS32
Gu	Do-Heon	626		Advancing serial crystallography: comparative analysis of low and high energy data collection	GROUND FLOOR	8	28 August, Wed.	MS03
Gierster	Gerald	627		Crystal structure and phase transition in orthorhombic FeSO4OH	FIRST FLOOR	49	27 August, Tue.	MS18 - Crystal-chemistry of minerals in the Universe: genesis, phase stability, and planetological implications
Granatino	Paola	628		Understanding ladderane biosynthesis: Towards structural and mechanistic insights from an anammox β -ketoacyl-ACP-synthase II	FIRST FLOOR	24	28 August, Wed.	MS06
Lamba	Doriano	629		acetylcholinesterase adduct formation and evolution: structural and mechanistic insights into an aged-like inactive complex susceptible to reactivation by a combination of nucleophiles	FIRST FLOOR	25	28 August, Wed.	MS06
Khachatryan	Hamlet	630	Conor Wild; Frank von Delft	DiffEMA: Diffusion-based generative network for protein model local quality assessment and auto-completion	GROUND FLOOR	23	27 August, Tue.	MS4 - AI, software developments and Machine learning applied to MX and CryoEM
Karothu	Durga Prasad	631		Exceptionally high work density of a ferroelectric dynamic organic crystal around room temperature	THIRD FLOOR	114	27 August, Tue.	MS28 - Structural characterization of Energy Harvesting and Conversion Materials
Wiggers	Christin	633		Diffuse scattering in Sanidines	FIRST FLOOR	80	28 August, Wed.	MS17
Bethanis	Kostas	635		Crystal Structure of Cannabidiol Inclusion Complexes in Native and Methylated beta-Cyclodextrins	THIRD FLOOR	114	29 August, Thur.	MS33
Motaln	Klemen	637	Kshitij Gurung; Petr Brázda; Lukáš Palatinus; Matic Lozinšek	Structural investigation of fluoridopalladates(IV) by 3D ED	GROUND FLOOR	23	29 August, Thur.	MS20
John	Sanjay	640	Roland Resel	Identification of a metastable phase and an unstable phase in 1,1'-Binaphthalene	FIRST FLOOR	101	27 August, Tue.	MS26 - Chirality: Meeting point of crystallography, chemistry and topology
Holczbauer	Tamás	641		The effect of high pressure on organocatalyst containing crystal structures	FIRST FLOOR	89	29 August, Thur.	MS27
Squeglia	Flavia	642	Valeria Napolitano	Crystallographic and functional studies of Kp-lin, a nano-sized protective cage from Klebsiella pneumoniae	FIRST FLOOR	31	29 August, Thur.	MS10
Barra	Giovanni	643		The molecular chaperone HtpG is a promising antigen against Mycobacterium tuberculosis	FIRST FLOOR	32	29 August, Thur.	MS10
Andreini	Antonio	644	Martina Lippi; Paola Paoli; Alessio Picchi; Patrizia Rossi	Further insights into the factors influencing the Anatase-Rutile Phase Transition for potential distributed temperature measurements	FIRST FLOOR	69	29 August, Thur.	MS25
Rouquette	Jerome	645		BaCo ₂ with Tetrahedral Cobalt Coordination: Unlocking Energy Storage and Conversion in BaCo ₂ - δ Materials	FIRST FLOOR	70	29 August, Thur.	MS25
Śmietańska-Nowak	Joanna	646		Application of advanced multidimensional analysis methods to study modulated structures of the Hyp-1/ANS protein complex	FIRST FLOOR	43	29 August, Thur.	MS14

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Dimitrova	Hristina	647		Co-crystallization of DNA Sequences, from the Promoter Regions of Genes Responsible for the Development of Degenerative Diseases, with Fluorescent Markers and Ligands	GROUND FLOOR	8	29 August, Thur.	MS01
Cioci	Gianluca	648		Structural enzymology for the synthesis and functionalization of biopolymers	FIRST FLOOR	26	28 August, Wed.	MS06
Díaz-Ramos	Isolina	649		Earth-based mortars in the built heritage: recovering the urban heritage of the Canary Islands, Spain	THIRD FLOOR	122	29 August, Thur.	MS36
Warren	Anna	650		The micro/nanofocus crystallography beamline VMXm at Diamond Light Source	GROUND FLOOR	9	28 August, Wed.	MS03
Duverger-Nédellec	Elen	651		Creation of a Young Crystallographers Section at the French Association of Crystallography	FIRST FLOOR	74	27 August, Tue.	MS37 - How to address questions, doubts and struggles of a young crystallographer
Kekez	Ivana	652		Mgy a novel metagenomic esterase as an excellent target for environment friendly degradation of polylactic acid	FIRST FLOOR	27	28 August, Wed.	MS06
Kascakova	Barbora	653		Targeting 3Cpro: A Promising Approach for Inhibiting Enterovirus D68	FIRST FLOOR	34	29 August, Thur.	MS10
Ciesielski	Arkadiusz	655	Anna Sadocha	Structural studies of urea clathrates with aliphatic monoamines	FIRST FLOOR	102	27 August, Tue.	MS26 - Chirality: Meeting point of crystallography, chemistry and topology
Ciesielski	Arkadiusz	656	Anna Sadocha	Structural studies of urea clathrates with aliphatic diamines	FIRST FLOOR	103	27 August, Tue.	MS26 - Chirality: Meeting point of crystallography, chemistry and topology
Ilkaeva	Marina	659		In situ PXRD studies of poly(heptazine imide)-based adsorbents	FIRST FLOOR	79	29 August, Thur.	MS30
Čejka	Jan	660		New Forms of Imatinib	THIRD FLOOR	145	28 August, Wed.	MS32
Putra	Okky	661		Unveiling dehydration and solid-solid phase transition through single crystal-to-single crystal transformation: A case study of AZD9898	THIRD FLOOR	140	29 August, Thur.	MS40
Lanza	Arianna	662		Anion-mediated solid-state polymerization of a simple Cu-bpy complex, investigated via electron diffraction	THIRD FLOOR	151	29 August, Thur.	MS29
Eigner	Václav	663		Temperature related bending of isothiuronium hippurate trihydrate crystals	THIRD FLOOR	115	29 August, Thur.	MS33
Koutska	Anna	664	Anna Koutska	Investigating the effect of neurodevelopmental disorder missense variants on cognitive function with Drosophila	GROUND FLOOR	14	28 August, Wed.	MS05
Havlickova	Petra	665	Anna Koutska; Ivana Kuta Smatanova; Michaela Fenckova	From Uncertainty to Molecular Mechanism: Missense Mutations in BRAF and MAP2K1 in Cognitive Disorders	GROUND FLOOR	15	28 August, Wed.	MS05
Raza	Arsez	666		Experimental demonstration of a second polymorph of Osmium acetylacetonate(III) by magnetometric technique.	FIRST FLOOR	90	28 August, Wed.	MS19
Reubold	Thomas	667		Crystal structure of the effector/metaeffector pair SidL/LegA11 from Legionella pneumophila	GROUND FLOOR	16	28 August, Wed.	MS05
Barbaro	Anna	668		Nanoscale investigation of extraterrestrial ureilic carbon	FIRST FLOOR	50	27 August, Tue.	MS18 - Crystal-chemistry of minerals in the Universe: genesis, phase stability, and planetological implications
Röhr	Caroline	669		Ca(Zn _{1-x} Cd _x) ₃ /5: Disorder models for known and new hexagonal intermetallics	FIRST FLOOR	44	29 August, Thur.	MS14
André	Vânia	670		The power of antibiotic coordination frameworks towards enhanced antimicrobial activity	THIRD FLOOR	152	29 August, Thur.	MS29
Chelazzi	Laura	671		Ranolazine: crystal structure determination and investigation of its metastable polymorphs	THIRD FLOOR	141	29 August, Thur.	MS40
Sobral Carvalho	Ana Carina	672		New hydrated salts of Sparfloxacin: a supramolecular synthon analysis	THIRD FLOOR	146	28 August, Wed.	MS32
Matković-Čalogović	Dubravka	673	Ivica Dilović	Robustness and stability of the L-carnosine copper(II) dimer. Coordinatively unsaturated sites of the high-temperature structure	THIRD FLOOR	116	29 August, Thur.	MS33

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Bereczki	Laura	675	Petra Bombicz; Kende Attila Béres; Éva Kovács; László Kótai	Which one is the right space group?	FIRST FLOOR	75	27 August, Tue.	MS37 - How to address questions, doubts and struggles of a young crystallographer
Benslimane	M.	676	Y. K. Redjel	Synthesis and structures of dimeric and polymeric carboxylates complexes of copper (II) and cobalt (II)	THIRD FLOOR	153	29 August, Thur.	MS29
Scatena	Rebecca	678		The materials and magnetism beamline, I16 at diamond light source Ltd	FIRST FLOOR	91	28 August, Wed.	MS19
Managutti	Praveen	683		Enhancing SOFC Anode Performance through Cerium and Nickel Doping in PrBaMn2O5+δ Structures	FIRST FLOOR	71	29 August, Thur.	MS25
Wicher	Barbara	685		Cocrystalline and co-amorphous systems of metformin with nonsteroidal anti-inflammatory drug meloxicam – synthesis, crystal structure and thermal properties	THIRD FLOOR	147	28 August, Wed.	MS32
Hofer	Gerhard	687		Protein serial electron diffraction for everyone	FIRST FLOOR	42	27 August, Tue.	MS15 - ED small waves, big ponds – Biomolecules and macromolecules
Lima	Gustavo Jones	688		Crystal Structure, Hirshfeld Surface Analysis and Spectroscopic Studies of Newly Synthesized Dithiocarbazate Pyrazole Compound	FIRST FLOOR	102	29 August, Thur.	MS31
Faye Diouf	Moussa D.	689		Structural Characterization of MOFs using Three Dimensional Electron Diffraction	THIRD FLOOR	154	29 August, Thur.	MS29
Fetah	Banaz	691		Understanding the compression behaviour of artemisinin	FIRST FLOOR	90	29 August, Thur.	MS27
Liermann	H.-P.	692		Status and new developments at the Extreme Conditions beamline (ECB, P02.2) PETRA III, DESY	FIRST FLOOR	91	29 August, Thur.	MS27
Kuzel	Radomir	693		Growth of thin films of hexaferrites prepared by chemical solution deposition	THIRD FLOOR	155	29 August, Thur.	MS29
Schleissner	Pamela	695		From Protein Dynamics to Biological Function: The Impact of LCLS-II and the Center for Structural Dynamics in Biology	FIRST FLOOR	62	27 August, Tue.	MS23 - Future of light sources and XFEL
Ruth	Paul Niklas	696		QCrBox: Unlocking (Quantum) Crystallography	FIRST FLOOR	52	28 August, Wed.	MS11
May	Zoltán	697		Portable handheld XRF and μ -XRD examination of a late Roman copper cauldron	THIRD FLOOR	123	29 August, Thur.	MS36
Oeffner	Robert	698		A Joint X-ray/cryo-EM platform for fragment-based drug discovery	FIRST FLOOR	56	29 August, Thur.	MS22
Antoniadis	Nadia	699	Thomas Braun; Nicolas Candia; Andreas Engel; Alejandro Lorca Moulliaa; Armin Ruf	The cryoWriter – a new and reliable way of automated cryo-EM grid preparation	GROUND FLOOR	15	29 August, Thur.	MS09
Konovalova	Iryna	700		Application of quantum chemistry methods to analyse supramolecular architecture of halogen substituted anilines	FIRST FLOOR	87	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography
Xu	Yizhi	701	Shaodi Li; Jiaoyan Xu; James Darby; Andrew J. Morris; Tomislav Friščić; Mihails Arhangeliskis	Mechanochemical synthesis and structural characterization of hexafluorosilicate containing MOFs	THIRD FLOOR	156	29 August, Thur.	MS29
Moncol	Jan	704		Crystal structure of new palladium(II) salicylate complexes with N,N-donor ligands	FIRST FLOOR	88	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography
Lucchini	Davide	715		Crystal structures of rhenium(V) complexes with thiosemicarbazonate ligands	FIRST FLOOR	44	28 August, Wed.	MS10