

FIRST AUTHOR'S LAST NAME	FIRST AUTHOR'S FIRST NAME	OTHER AUTHORS' NAMES	TITLE	POSTER ID	FLOOR	PANEL NR.	DAY	SESSION
Adjimani	Joseph	Laszlo Fabian; Yaroslav Khimyak	Balancing Act: Studying Stoichiometry in Hydroxybenzoic Acid-Cyclic Amide Cocrystals with X-Ray Diffraction and In-situ solid state NMR	521	THIRD FLOOR	141	28 August, Wed.	MS32
Agarwal	Harshit		Charge density wave structural phase transition in SrAl ₂ Ga ₂	430	FIRST FLOOR	39	29 August, Thur.	MS14
Aghaei Hakkak	Rouzbah		(CN5H 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	481	FIRST FLOOR	76	28 August, Wed.	MS17
Aguiar Suescun	Ivana	Natalia Alvarez; Valentina Costa; Isabel Galain; Emiliano García; Ayleen Grenni; Noelia Méndez; Florencia Menéndez; Federico Mesa; Maia Mombrú; Ivana Núñez; Santiago Ploli; Carlos Rojas; Leopoldo Suescun; Santiago Valiero; Martina Viera; Carlos Yáñez	CNCC - Concurso Nacional de Crecimiento de Cristales de Uruguay: 10 years of a successful crystal growing competition for schoolchildren and more.	591	THIRD FLOOR	140	27 August, Tue.	MS41 - Approaches and tools for learning crystallography efficiently and avoiding misconceptions
Alberto	Roger	Roger Alberto; Vladimir Azov; Alice Brink; Dumisani Kama; Andreas Roodt	Exploring Novel Organometallic Compounds: Bridging Catalysis and Medicine through Crystallographic Insights	93	FIRST FLOOR	63	27 August, Tue.	MS33 - Correlate molecular structure with materials properties
Alexander	Orbett		Metallo-organic chemistry of inert d ₆ -low spin ReI-tricarbonyl synthon	426	FIRST FLOOR	70	27 August, Tue.	MS33 - Correlate molecular structure with materials properties
Ali	Areesha	Vanessa Cascos; Stewart Clark; Manon Jones; Emma McCabe	Structure-composition relationships in layered perovskite-related materials	39	THIRD FLOOR	144	27 August, Tue.	MS29 - Structural characterization in Functional materials
Alotaibi	Thamer		A systematic study of crystal size influence on Crystal Sponge experiment outcomes	158	THIRD FLOOR	129	28 August, Wed.	MS30
Anae	Madden	Lars Ehm	Laser-heated rapid decompression of enstatite (Mg ₂ Si ₂ O ₆): Constraining impact barometry	377	FIRST FLOOR	46	27 August, Tue.	MS18 - Crystal-chemistry of minerals in the Universe: genesis, phase stability, and planetological implications
Andersen	Asser Sloth	Frederik Flindt Kreiner; František Hubálek; Eva Johansson; Thomas Kjeldsen; Peter Kurtzhals; Gerd Schluckebier	Application of structural insights in the molecular engineering of insulin for recombinant expression in yeast.	311	FIRST FLOOR	26	29 August, Thur.	MS10
André	Vânia		The power of antibiotic coordination frameworks towards enhanced antimicrobial activity	670	THIRD FLOOR	152	29 August, Thur.	MS29
Andreeva	Elena A.		Discovery of a novel iron-copper-sulfur cluster in a glucose-methanol-choline (GMC) oxidoreductase	236	FIRST FLOOR	39	27 August, Tue.	MS6 - Structural studies in Enzymology
Andreini	Antonio	Martina Lippi; Paola Paoli; Alessio Picchi; Patrizia Rossi	Further insights into the factors influencing the Anatase-Rutile Phase Transition for potential distributed temperature measurements	644	FIRST FLOOR	69	29 August, Thur.	MS25
Anosova	Olga	Vitaliy Kurlin	Richard Feynman's visual hint gave birth to a new area of continuous crystallography	493	SECOND FLOOR	106	29 August, Thur.	MS38
Antoniadis	Nadia	Thomas Braun; Nicolas Candia; Andreas Engel; Alejandro Lorca Moullia; Armin Ruf	The cryoWriter – a new and reliable way of automated cryo-EM grid preparation	699	GROUND FLOOR	15	29 August, Thur.	MS09
Arhangelskis	Mihails	Sibananda Dash	Parameterization of an intermolecular forcefield for halogen bonded molecular crystals	411	FIRST FLOOR	98	29 August, Thur.	MS31
Arletti	Rossella	Riccardo Fantini; Michael Fischer; Monica Argenziano; Roberta Cavalli; Lorenzo Mino	Enhanced Photostability and Efficacy of Hybrid Zeolite-Encapsulated UV Filters for Sunscreen Applications	266	THIRD FLOOR	114	28 August, Wed.	MS29
Atamas	Anastasiia		Investigation of the molecular architecture of Candida auris ribosome	163	GROUND FLOOR	12	29 August, Thur.	MS09
Bae	Euiyoung	Hyejin Oh	Crystal structure of GajB protein in Gabija anti-phage defense	20	FIRST FLOOR	31	27 August, Tue.	MS6 - Structural studies in Enzymology
Baisch	Ulrich		Ion-induced cocrystallisation and polymorph Screening	580	THIRD FLOOR	139	29 August, Thur.	MS40
Balasingham	Jonathan	Vitaliy Kurlin; Viktor Zamaraev	Applications of isometry invariants on material property prediction	348	FIRST FLOOR	68	27 August, Tue.	MS33 - Correlate molecular structure with materials properties
Baldock	Peter	Stefan Kolek; Patrick Shaw Stewart; Jack Stubbs	Sample preparation for routine and advanced structural biology, including serial data collection and microED	15	GROUND FLOOR	6	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature

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Banerjee	Arpan		Biochemical and structural insights on pH-dependent cooperativity of glutamate dehydrogenase in <i>Saccharomyces cerevisiae</i>	285	FIRST FLOOR	41	27 August, Tue.	MS6 - Structural studies in Enzymology
Barbaro	Anna		Nanoscale investigation of extraterrestrial ureilitic carbon	668	FIRST FLOOR	50	27 August, Tue.	MS18 - Crystal-chemistry of minerals in the Universe: genesis, phase stability, and planetological implications
Barra	Giovanni		The molecular chaperone HtpG is a promising antigen against <i>Mycobacterium tuberculosis</i>	643	FIRST FLOOR	32	29 August, Thur.	MS10
Batisai	Eustina		Gas sorption studies of mixed ligand metal-organic frameworks containing substituted diimide ligands	36	THIRD FLOOR	126	28 August, Wed.	MS30
Batmanghelich	Shiva	Andrzej Katrusiak; Jakub Kaczowski; Iwona Plowas-Korus	Resorcinol polymorphism: the lattice energy and conformers	148	SECOND FLOOR	104	28 August, Wed.	MS27
Bauer	Melanie	Ute Kolb	Structure elucidation of two different materials with TADF properties using three-dimensional electron diffraction	354	THIRD FLOOR	121	28 August, Wed.	MS29
Benkanoun	Aouaouche		Structural description and thermal analysis of a new diphenate 1D coordination polymer	116	THIRD FLOOR	150	27 August, Tue.	MS29 - Structural characterization in Functional materials
Benslimane	M.	Y. K. Redjel	Synthesis and structures of dimeric and polymeric carboxylates complexes of copper (II) and cobalt (II)	676	THIRD FLOOR	153	29 August, Thur.	MS29
Benzitouni	Ines		Investigations of the biological activity of new sulfanilamide derivative: single crystal X-ray diffraction analysis, DFT computational, in-silico ADME and molecular docking studies.	141	THIRD FLOOR	152	27 August, Tue.	MS29 - Structural characterization in Functional materials
Bereczki	Laura	Petra Bombicz; Sourav De; Gabriella Győrík; Tamás Holczbauer; Nóra Veronika May; András Tompos; Zoltán Varga; András Wacha	Curious Chemist summer camp at the Research Centre for Natural Sciences in Hungary	520	THIRD FLOOR	138	27 August, Tue.	MS41 - Approaches and tools for learning crystallography efficiently and avoiding misconceptions
Bereczki	Laura	Petra Bombicz; Kende Attila Béres; Éva Kováts; László Kótai	Which one is the right space group?	675	FIRST FLOOR	75	27 August, Tue.	MS37 - How to address questions, doubts and struggles of a young crystallographer
Bethanis	Kostas		Crystal Structure of Cannabidiol Inclusion Complexes in Native and Methylated beta-Cyclodextrins	635	THIRD FLOOR	114	29 August, Thur.	MS33
Bhattacharya	Suman		Multicomponent crystals of sulfamic acid with amino acids as alternative piezoelectric / NLO materials	22	THIRD FLOOR	116	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Biran	Ido	Alexei Bosak; Zuo-Guang Ye; Igor Levin; Semën Gorfman	Lattice match between coexisting cubic and tetragonal phases in PMN-PT at the phase transition	462	THIRD FLOOR	144	29 August, Thur.	MS29
Bistrović	Andrea	Silvana Raić-Malić; Mario Cetina	Structures and biological properties of mono- and bis-pseudopurines	256	FIRST FLOOR	67	27 August, Tue.	MS33 - Correlate molecular structure with materials properties
Bjelcic	Monika		Introducing MicroMAX: Advanced Beamline for Serial Crystallography and Time-Resolved Studies	296	GROUND FLOOR	13	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
Blaha	Jan		Efficient enrichment of in cellulose grown protein crystals	12	FIRST FLOOR	34	28 August, Wed.	MS10
Bogdanovic	Milica	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	142	THIRD FLOOR	153	27 August, Tue.	MS29 - Structural characterization in Functional materials
Bogdanović	Milica		Pd(II) and Pt(II) complexes with N-benzylphenotiazine – Hirshfeld atom refinement and intermolecular interaction energies	115	FIRST FLOOR	49	28 August, Wed.	MS11
Bolton	Rachel	Robin Owen; Ivo Tews	SSX and SFX probe the cyanobacterial F ₁ A iron binding protein by X-ray induced photoreduction and reveal a switch for Fe(II) / Fe(III) binding	417	GROUND FLOOR	3	28 August, Wed.	MS03
Bombicz	Petra		Noncovalent interactions – an obscure aspect of the definition of isostructurality	299	FIRST FLOOR	95	29 August, Thur.	MS31
Borovina	Mladen	Ivan Kodrin; Mateja PISAČIĆ; Matteo Zausnig; Marijana Đaković	Mechanoflexibility in crystalline coordination polymers: Correlating mechanical properties with structural prerequisites and consequences	556	THIRD FLOOR	110	29 August, Thur.	MS33
Bortel	Tyler	Peter Moeck	Detecting and Correcting Systematic STM Imaging Errors: Plane Symmetry of Graphite Calibration Samples	270	FIRST FLOOR	84	28 August, Wed.	MS19

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Boucherabine	Djihed		Copper complexes of new unsymmetrically NNOO ligands: X-ray structure, NLO properties, catalytic oxidation and bromoperoxidase activities	6	THIRD FLOOR	115	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Boullay	Philippe	Sara Passuti; Adrian David; Emmanuel GUILMEAU	Crystal structures at the nanoscale with Scanning Electron Diffraction Tomography	390	FIRST FLOOR	59	28 August, Wed.	MS16
Bramantya	Bramantya		Ab initio crystal structure prediction (CSP) of magnetic metal-organic frameworks (MOFs)	505	FIRST FLOOR	88	28 August, Wed.	MS19
Braun	Maxime		Anti-magnetolectricity, a hidden order probed by Dynamical Magnetic Charges	503	FIRST FLOOR	87	28 August, Wed.	MS19
Breen	Olivia		Synthesis of iron- and lithium- based oxalate compounds for use as cathode materials	77	THIRD FLOOR	146	27 August, Tue.	MS29 - Structural characterization in Functional materials
Brown	Stephen		Photoinitiated Single-Crystal to Single-Crystal Redox Transformations of Titanium-Oxo Clusters	206	FIRST FLOOR	81	28 August, Wed.	MS19
Brůx	Daniel	Florian Kleemiss	Creation and Analysis of a Single Crystal X-ray Diffraction Experiment Benchmark Database	328	FIRST FLOOR	72	27 August, Tue.	MS37 - How to address questions, doubts and struggles of a young crystallographer
Bu	Kejun	Yang Ding; Hazohe Liu; Xujie Lü; Anna Moliterni; Takeshi Nakagawa; Jasminka Popović; Martina Vrankić	Structure-property behaviour of $N(C_2H_5)_3CH_3FeBr_4$ powder under high pressure	352	FIRST FLOOR	81	29 August, Thur.	MS27
Bugański	Ireneusz		The impact of orbitals interactions on the stability of ZnMgSc approximant crystal	387	FIRST FLOOR	37	29 August, Thur.	MS14
Burian	Max	Tilman Donath; Sascha Grimm; Sofia Trampari	PILATUS4 Hybrid Photon Counting Detectors for Efficient and Fast X-ray Diffraction	210	FIRST FLOOR	92	28 August, Wed.	MS24
Butler	Abbey		Understanding the molecular basis of retinoid signalling	52	FIRST FLOOR	37	28 August, Wed.	MS10
Byun	Sujeong	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>	100	FIRST FLOOR	37	27 August, Tue.	MS6 - Structural studies in Enzymology
Cabaj	Malgorzata		Exploring the influence of imperfections on 3D electron diffraction intensities through multislice simulations	397	FIRST FLOOR	61	28 August, Wed.	MS16
Cagossi	Giorgio	Andrea Daolio	A novel family of hexanuclear macromolecular complexes obtained under ball-milling conditions	94	THIRD FLOOR	147	27 August, Tue.	MS29 - Structural characterization in Functional materials
Calora	Alessia	Matteo Calvaresi; Matteo Di Giosia; Giuseppe Falini; Silvia Fanti; Simona Fermani; José Gavira; Daniele Tedesco	BSA nanoparticles as innovative heterogeneous nucleants for protein crystallization	76	GROUND FLOOR	9	29 August, Thur.	MS08
Carlini	Lavinia		Protein Targeting to Glycogen (PTG), a validated target in Lafora disease	33	FIRST FLOOR	35	28 August, Wed.	MS10
Carloni	Giacomo	Quentin Gaday	Structural insights into cell septation in <i>Mycobacterium tuberculosis</i>	369	GROUND FLOOR	4	27 August, Tue.	MS02 - Hot structures
Castiglione	Franca	Stefano Elli; Antonino Famulari; Javier Marti Rujas; Alessandro Zanotti	Molecular recognition of aromatics in spherical nanocages	196	THIRD FLOOR	130	28 August, Wed.	MS30
Catapano	Lucrezia		Enhancing structural refinement of macromolecules obtained from neutron crystallography	613	FIRST FLOOR	28	28 August, Wed.	MS06
Cazzola	Davide	Davide Cazzola; Christoph Mueller-Dieckmann; Ehmke Pohl	Targeting the sphingolipid biosynthesis pathway of protozoan parasites as drug targets	51	FIRST FLOOR	24	27 August, Tue.	MS5 - Infectious and Neglected diseases
Ceborska	Magdalena		3,4-disubstituted benzoic acids as cofomers in the salts and cocrystals of pyrimethamine	191	THIRD FLOOR	123	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Čejka	Jan		New Forms of Imatinib	660	THIRD FLOOR	145	28 August, Wed.	MS32
Čerpakovska	Zane		Additive assisted mechanochemical control of caffeine:anthranilic acid co-crystal polymorphs	58	THIRD FLOOR	148	28 August, Wed.	MS40

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Cesselli	Daniela	Marta S. Semrau; Paola Storici	ULK1 inhibition for autophagy deregulation recovery	492	FIRST FLOOR	29	29 August, Thur.	MS10
Chakraborty	Atreyi	AMadhusudhan M.S	A genome-wide in-silico motif scan to identify functional clustering	365	GROUND FLOOR	4	29 August, Thur.	MS01
Chandra	Mohit		Investigation of structural correlations at dielectric and magnetic ordering in Cr/Fe doped alpha-Mn2O3	439	THIRD FLOOR	142	29 August, Thur.	MS29
Chelazzi	Laura		Ranolazine: crystal structure determination and investigation of its metastable polymorphs	671	THIRD FLOOR	141	29 August, Thur.	MS40
Chen	Shih-Lun		Theoretical and Experimental Investigations of X-ray Back Diffraction at Grazing Incidence	380	FIRST FLOOR	59	27 August, Tue.	MS23 - Future of light sources and XFEL
Chernyshov	Dmitry		Effect of X-ray radiation on structure and properties of molecular crystals: from damage to a fine tuning	239	FIRST FLOOR	66	27 August, Tue.	MS33 - Correlate molecular structure with materials properties
Chinellato	Monica		Class IIa HDAC derived peptides elucidate the promiscuous binding to myocyte enhancer factor-2 in complex with DNA	592	FIRST FLOOR	30	29 August, Thur.	MS10
Chintakindi	Hrushikesh	Lukas Palatinus	Analysing the frame scaling and orientation matrix in the presence of appreciable dynamic diffraction effects utilizing simulated 3D ED data	567	FIRST FLOOR	66	28 August, Wed.	MS16
Cholakova	Diana	Nikolai Denkov; Slavka Tcholakova	Polymorphism in triglyceride systems: in bulk and in emulsion droplets	575	THIRD FLOOR	138	29 August, Thur.	MS40
Chrappan Soldavini	Benedetta		New ring-structured high pressure and temperature CaSiO3 polymorph and its stability field	34	FIRST FLOOR	89	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Cianci	Michele		Unravelling the mechanism of lipid – enzyme interactions in the limbus region of lipases at atomic resolution	384	GROUND FLOOR	20	28 August, Wed.	MS06
Ciesielski	Arkadiusz	Anna Sadocha	Structural studies of urea clathrates with aliphatic monoamines	655	FIRST FLOOR	102	27 August, Tue.	MS26 - Chirality: Meeting point of crystallography, chemistry and topology
Ciesielski	Arkadiusz	Anna Sadocha	Structural studies of urea clathrates with aliphatic diamines	656	FIRST FLOOR	103	27 August, Tue.	MS26 - Chirality: Meeting point of crystallography, chemistry and topology
Cioci	Gianluca		Structural enzymology for the synthesis and functionalization of biopolymers	648	FIRST FLOOR	26	28 August, Wed.	MS06
Clarke	Brendan		Applications of precession-assisted scanned nanobeam diffraction tomography to sample metrology over large ROIs	477	FIRST FLOOR	64	28 August, Wed.	MS16
Clough	Lewis		The high pressure behaviour of Nd(XeF2)3(TaF6)3	407	FIRST FLOOR	82	29 August, Thur.	MS27
Coles	Simon J	Peter Horton	Hands-on, challenge-based teaching in crystallography undergraduate practicals	170	THIRD FLOOR	135	27 August, Tue.	MS41 - Approaches and tools for learning crystallography efficiently and avoiding misconceptions
Coles	Simon		Raw Data Letters - describing and publishing raw diffraction data in a FAIR way	612	THIRD FLOOR	126	29 August, Thur.	MS38
Cormack	Isabel	Ehmke Pohl; Bernd Striberny	Fantastic SSBs and where to find them	71	GROUND FLOOR	1	29 August, Thur.	MS01
Crichton	Wilson		The EBS large volume press facility at the ESRF	479	FIRST FLOOR	84	29 August, Thur.	MS27
Crowley	Peter		Protein assembly and crystallization with synthetic macrocycles	625	THIRD FLOOR	144	28 August, Wed.	MS32
Curtis	Esther		Anisotropy of Oxide Ion Conductors	153	THIRD FLOOR	107	27 August, Tue.	MS28 - Structural characterization of Energy Harvesting and Conversion Materials
Dadivanyan	Natalia	Lei Ding; Gwilherm Nénert; Maria Orlova	Crystallization of molecular glass: from amorphous state to new polymorphic forms in the API sodium naproxen	272	THIRD FLOOR	153	28 August, Wed.	MS40
Danylyuk	Oksana	Oksana Danylyuk	Host-guest interactions guide pentamidine folding inside and outside the cavities of macrocyclic hosts	183	THIRD FLOOR	132	27 August, Tue.	MS31 - Noncovalent interactions in structure design

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Day	Maxwell		RamanCrystalHunter: a new program and database for processing, analysis, and identification of Raman spectra	416	FIRST FLOOR	47	27 August, Tue.	MS26 - Crystal chemistry of minerals in the Universe: genesis, phase stability, and planetological implications
De	Sourav		The effect of high pressure on the crystal structure of organocatalysts	586	FIRST FLOOR	88	29 August, Thur.	MS27
De Felice	Sofia		Structural and functional characterization of hyper-stable human serum albumin variants	221	FIRST FLOOR	24	29 August, Thur.	MS10
de Sanctis	Daniele		Serial Microsecond Crystallography at ESRF-EBS	238	GROUND FLOOR	11	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
DeBorggraeve	Wim	Jochin Demaerel; Ermal Ismalaj; Bingyu Li; Kexin Su; Luc VanMeervelt; Steven Verhelst	Ex situ Generation of Thiazyl Trifluoride (NSF3) as a Gaseous SuFEx Hub	98	FIRST FLOOR	40	28 August, Wed.	MS10
Dejoie	Catherine		Correcting the axial divergence from high-resolution powder diffraction data	353	FIRST FLOOR	95	28 August, Wed.	MS24
Del Giudice	Alessandra	Libero Gurreri; Paolo Trost; Roberto Marotta; Francesca Sparla; Simona Fermani	Regulation pathway of photosynthetic glyceraldehyde 3-phosphate dehydrogenase	456	GROUND FLOOR	21	28 August, Wed.	MS06
Derese	Solomon	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	589	THIRD FLOOR	139	27 August, Tue.	MS41 - Approaches and tools for learning crystallography efficiently and avoiding misconceptions
Deresz	Krystyna		Nitro-to-endo-nitrito isomerization in the solid state: unravelling light-induced mechanism of the process	64	FIRST FLOOR	57	29 August, Thur.	MS25
Dialpuri	Jordan		NucleoFind: A Deep-Learning Network for Interpreting Nucleic Acid Electron Density	304	GROUND FLOOR	3	29 August, Thur.	MS01
Diaz-Ramos	Isolina		Earth-based mortars in the built heritage: recovering the urban heritage of the Canary Islands, Spain	649	THIRD FLOOR	122	29 August, Thur.	MS36
Dimitrova	Hristina		Co-crystallization of DNA Sequences, from the Promoter Regions of Genes Responsible for the Development of Degenerative Diseases, with Fluorescent Markers and Ligands	647	GROUND FLOOR	8	29 August, Thur.	MS01
Dohnálek	Jan	Tomáš Kovář; Natašja Borić; Petra Šedláková; Barbora Brezovská; Hana Šaňderová; Alena Křeneková; Martin Hubálek; Mária Trundová; Kristýna	A novel mechanism of bacterial transcription initiation under HelD-mediated protection	279	GROUND FLOOR	2	29 August, Thur.	MS01
Dolomanov	Oleg		Olex2 and olex2.refine	303	FIRST FLOOR	56	28 August, Wed.	MS16
Dranka	Maciej		Utilizing structural studies for developing a new concept of aqueous electrolytes based on lithium 4,5-dicyanoimidazolate hydrates	568	THIRD FLOOR	111	29 August, Thur.	MS33
Du	Chao-Hung		Study of the electronic ordering in quantum materials of RbV3Sb5 and Ir2In8Se	102	FIRST FLOOR	35	29 August, Thur.	MS14
Du	Chao-Hung		Study of the electronic ordering in quantum materials of RbV3Sb5 and Ir2In8Se	223	THIRD FLOOR	110	28 August, Wed.	MS29
Dudek	Marta	Agata Jeziorna; Przemysław Nowak; Dineshchakravarthy Senthurpandi	Rich polymorphic landscape of binary systems of meloxicam with imidazole and pyrazole	373	THIRD FLOOR	154	28 August, Wed.	MS40
Duverger-Nédellec	Elen		Creation of a Young Crystallographers Section at the French Association of Crystallography	651	FIRST FLOOR	74	27 August, Tue.	MS37 - How to address questions, doubts and struggles of a young crystallographer
Ebel	Ben		First implementation of tight-binding methods (xtb) for quantum crystallographic refinement	327	THIRD FLOOR	131	29 August, Thur.	MS39
Edkins	Katharina		Exploring co-crystallisation as a technique for taste-masking of nevirapine	91	THIRD FLOOR	119	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Edwards	Matthew	Mark Senn	Restoring superconductivity in hole-doped Pr2CuO4 via high-pressure phase transitions	251	THIRD FLOOR	113	28 August, Wed.	MS29
Eigner	Václav		Temperature related bending of isothiuronium hippurate trihydrate crystals	663	THIRD FLOOR	115	29 August, Thur.	MS33
Ellaway	Joseph		Advancing protein conformation analysis: A comprehensive clustering pipeline for the Protein Data Bank	312	FIRST FLOOR	51	29 August, Thur.	MS22

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Elliott	Luc		Slice'N'Dice: Maximising the value of predicted models for structural biologists	461	FIRST FLOOR	53	29 August, Thur.	MS22
Esegood	Mark R.J.		3D ED and Synchrotron Radiation SCXRD Combine to Solve a Drug Identification Puzzle	344	FIRST FLOOR	56	27 August, Tue.	MS20 - When can ED challenges XRD in small molecule crystallography?
Engel	Katja	Thomas Schleid	Rb ₄ [As ₂ S ₁₀]: A Rubidium Polythioarsenate(V) with an Unusual Discrete [S ₃ As ₅ (S ₂)As ₅ S ₃] ₄ - Anion	247	THIRD FLOOR	112	28 August, Wed.	MS29
Ernst	Michelle		From capture to catalysis: Insights from atomistic simulations into MOF and COF host-guest interactions and guest dynamics	88	FIRST FLOOR	48	28 August, Wed.	MS11
Esrifili	Leili	Christophe M.L. Vande Velde	Hydrogen bond donating MOFs - synthesis and structure	381	THIRD FLOOR	134	28 August, Wed.	MS30
Etter	Martin		The Powder Diffraction and Total Scattering Beamline P02.1 at PETRA III, DESY	288	FIRST FLOOR	93	28 August, Wed.	MS24
Fahl	Benjamin		An all-order phonon approach to thermal diffuse scattering	295	FIRST FLOOR	31	28 August, Wed.	MS35
Fando	Maria	Wenwei Cao; Pierre-Loïc Savary; Victor Castaing;	Demystifying CCP4 Cloud concepts: safeguarding structure determination through data structure and automation	233	THIRD FLOOR	129	29 August, Thur.	MS39
Fang	Xue	Ana Becerra; Cécile Genevois; Emmanuel Veron; Didier Zanghi; Matthew Dyer; Alessio Zandonà;	Synthesis and structure of highly non-stoichiometric garnets RE ₃ +xAl ₅ -xO ₁₂ (0 < x < 0.6)	109	THIRD FLOOR	149	27 August, Tue.	MS29 - Structural characterization in Functional materials
Faye Diouf	Moussa D.		Structural Characterization of MOFs using Three Dimensional Electron Diffraction	689	THIRD FLOOR	154	29 August, Thur.	MS29
Fetah	Banaz		Understanding the compression behaviour of artemisinin	691	FIRST FLOOR	90	29 August, Thur.	MS27
Folkers	Laura		Open the black box with X-Area's intuitive, interactive, and colourful data quality assessment graphics	203	THIRD FLOOR	128	29 August, Thur.	MS39
Folkers	Laura		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	204	THIRD FLOOR	136	27 August, Tue.	MS41 - Approaches and tools for learning crystallography efficiently and avoiding misconceptions
Fonjallaz	Alexis		Parameter optimization for serial diffraction data analysis	146	FIRST FLOOR	47	29 August, Thur.	MS22
Francia	Nicholas		Comparison of crystal structure similarity algorithms and analysis of large sets of theoretically predicted structures	515	FIRST FLOOR	55	29 August, Thur.	MS22
Freitag-Pohl	Stefanie		Protein-Ligand Interactions with the Dianthus Screening Platform	334	FIRST FLOOR	27	27 August, Tue.	MS5 - Infectious and Neglected diseases
Friedl	Sebastian		Pressure induced phase transition of [Ni(Tp*)(acac)(MeCN)]	74	FIRST FLOOR	98	28 August, Wed.	MS27
Friedly	Alexandra		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	444	THIRD FLOOR	143	29 August, Thur.	MS29
Friese	Karen		Incommensurate structures and radiation damage in K ₂ V ₃ O ₈ and Rb ₂ V ₃ O ₈ mixed-valence vanadate fresnoites	581	FIRST FLOOR	42	29 August, Thur.	MS14
Friggeri	Laura	William Midgley; Ehmke Pohl; Bojana Popovic	Optimising GOLD pipelines for in silico PROTAC screening	63	FIRST FLOOR	38	28 August, Wed.	MS10
Fuentes-Montero	Luis	David Waterman; Gwyndaf Evans	Dui2, the new graphical user interface for Dials	350	GROUND FLOOR	18	27 August, Tue.	MS4 - AI, software developments and Machine learning applied to MX and CryoEM
Gabellini	Giuseppe		Alcohol Dehydrogenases as model enzymes to investigate nucleotide cofactor specificity	82	FIRST FLOOR	35	27 August, Tue.	MS6 - Structural studies in Enzymology
Gabriele	Federica	Federica Gabriele	Structural characterization of thioredoxin reductase from <i>Cryptosporidium parvum</i> and its interaction with aurano-fin	370	FIRST FLOOR	28	27 August, Tue.	MS5 - Infectious and Neglected diseases

FIRST AUTHOR'S LAST NAME	FIRST AUTHOR'S FIRST NAME	OTHER AUTHORS' NAMES	TITLE	POSTER ID	FLOOR	PANEL NR.	DAY	SESSION
Ganesh	Bera		Structural Stability and Adsorption Behaviour of CO ₂ -Loaded Pure Silica CHA Zeolite under High Pressure conditions	291	FIRST FLOOR	80	29 August, Thur.	MS27
Ganguly	Sudakshina		AlphaFold Database and its impact on the crystallographic world	107	FIRST FLOOR	41	28 August, Wed.	MS10
Gao	Yunyun		A Robust Beamstop Shadow Outlier Rejection: Combining Crystallographic Statistics with Modern Clustering Method	504	FIRST FLOOR	54	29 August, Thur.	MS22
Garcia-Granda	Santiago		Pigments based in M ₂ SiO ₄ (M = Ni, Co) olivine solid solutions from SiO ₂ – rich compositions	216	FIRST FLOOR	91	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Garriga	Damià		Scientific opportunities for SSX in MX beamlines at ALBA	340	GROUND FLOOR	14	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
Gašparíková	Dorota		Glucokinase and structure-based drug discovery	465	FIRST FLOOR	28	29 August, Thur.	MS10
Gasser	Fabian		On the Lorentz correction for grazing incidence X-ray diffraction	228	SECOND FLOOR	105	29 August, Thur.	MS38
Gateshki	Milen	Thomas Dortmann; Thomas Degen; Mustapha Sadki; Nicholas Norberg; Gwilherm Nenert	The effect of sample displacement in X-ray powder diffraction measurements with laboratory diffractometers	347	FIRST FLOOR	94	28 August, Wed.	MS24
Gatta	G. Diego		Structural evolution and pressure-driven phase transitions in hydrated borates	112	FIRST FLOOR	90	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Gatta	G. Diego		(P,T)-behavior of an intermediate scapolite of unusual I4/m symmetry	343	FIRST FLOOR	45	27 August, Tue.	MS18 - Crystal-chemistry of minerals in the Universe: genesis, phase stability, and planetological implications
Gatto	Claudia Cristina		Structural Design, Hirshfeld Analysis And Noncovalent Interactions Of Newly Synthesized Ni(II) Complex With A Dithiocarbazate Ligand	89	THIRD FLOOR	127	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Gauffre	Pierre		Crystallographic structure of whole nsp14 from SARS-CoV-2 stabilised by a nanobody	86	FIRST FLOOR	36	27 August, Tue.	MS6 - Structural studies in Enzymology
Gemrich Hernández	Laura	Ute Kolb	Multi-method study of calcium-aluminate cement hydration and its crystal structures	297	FIRST FLOOR	76	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Gesing	Thorsten M.		Determination of the average crystallite size and the crystallite size distribution: The envelope function approach EnvACS	457	FIRST FLOOR	70	28 August, Wed.	MS17
Giester	Gerald		Crystal structure and phase transition in orthorhombic FeSO ₄ OH	627	FIRST FLOOR	49	27 August, Tue.	MS18 - Crystal-chemistry of minerals in the Universe: genesis, phase stability, and planetological implications
Gilski	Mirosław		Unusual helical crystal packing of potassium-independent L-asparaginase from <i>Phaseolus vulgaris</i>	255	GROUND FLOOR	14	29 August, Thur.	MS09
Gjørup	Frederik		Real-time data analysis at the DanMAX materials science beamline	317	FIRST FLOOR	63	29 August, Thur.	MS25
Gladyshevskii	Roman	Svitlana Pukas	Quaternary compounds in R–T–Al–M systems	399	THIRD FLOOR	123	28 August, Wed.	MS29
Gladyshevskii	Roman	Yaroslav Tokaychuk Ivanana Klemenčova, Vlad Depmeier, Sergey V. Krivovichev; Michael Czank; Marco Schowalter; Lukas Palatinus; Ira V. Rozhdresvnskaya; Viktor N.	Crystal structures of the phases in the systems T ₅ M ₃ –T ₅ M' ₃ (T = Ti, Zr, Hf; M = Al, Ga; M' = Si, Ge, Sn, Pb, Sb, Bi)	538	THIRD FLOOR	147	29 August, Thur.	MS29
Goetz	Emila		Eveslogite – a highly complex nanotubular titanosilicate mineral solved by 3D ED	447	FIRST FLOOR	68	28 August, Wed.	MS17
Gollé-Leidreiter	Philipp		The crystal structures of two Y ₂ O ₃ and B ₂ O ₃ containing pyroxenes	554	FIRST FLOOR	79	28 August, Wed.	MS17
Golz	Christopher	Anna Krawczuk	Spironolactone Polymorphism: Do New Methods Yield New Insights?	220	THIRD FLOOR	151	28 August, Wed.	MS40
Gonen	Tamir	Jieye Lin; Johan Unge	Automated MicroED as a powerful powder diffraction tool for complex samples	494	GROUND FLOOR	20	29 August, Thur.	MS20

FIRST AUTHOR'S LAST NAME	FIRST AUTHOR'S FIRST NAME	OTHER AUTHORS' NAMES	TITLE	POSTER ID	FLOOR	PANEL NR.	DAY	SESSION
Gorelik	Tatiana E.	Martin U. Schmidt	Stacking-disordered structure of Pigment Orange 13 (C32 H24 Cl2 N8 O2) from electron diffraction	273	FIRST FLOOR	29	28 August, Wed.	MS35
Götz	Emilia		Exploring new features in sub-micron crystal structure analysis with the XtaLAB Synergy-ED	536	FIRST FLOOR	65	28 August, Wed.	MS16
Grabowsky	Simon		The untold story of the world's most common crystal structure	194	FIRST FLOOR	85	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography
Granatino	Paola		Understanding ladderane biosynthesis: Towards structural and mechanistic insights from an anammox β -ketoacyl-ACP- synthase II	628	FIRST FLOOR	24	28 August, Wed.	MS06
Grineva	Olga		Comparative analysis of the magnetic properties of organic compounds without metal atoms and their molecular and crystal structures	590	THIRD FLOOR	112	29 August, Thur.	MS33
Gruene	Tim		Assignment of partial charges with 3D ED	62	FIRST FLOOR	82	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography
Gruene	Tim	Jeroen Anton van Bokhoven	Direct quantification of Aluminum content in zeolites by Three-Dimensional Electron Diffraction	286	FIRST FLOOR	55	28 August, Wed.	MS16
Grybauskas	Algirdas		Method of extending rotamer libraries and its usage in protein active site studies	463	GROUND FLOOR	22	28 August, Wed.	MS06
Grzeškiewicz	Anita		Solid-to-solid phase transitions in two isostructural Bi(III) complexes and their solid solution.	219	THIRD FLOOR	150	28 August, Wed.	MS40
Gu	Do-Heon		Advancing serial crystallography: comparative analysis of low and high energy data collection	626	GROUND FLOOR	8	28 August, Wed.	MS03
Gurung	Kshitij	Klemen Motaln; Matic Belak Vivod	Solving ambiguities: redetermining the crystal structures of rare Ag(I) compound using 3DED	192	FIRST FLOOR	53	27 August, Tue.	MS20 - When can ED challenges XRD in small molecule crystallography?
Hakala	B. Viliam	Sophia Kurig; Nicolas Walte; Karen Friese; Andrzej Grzechnik	Phase stability of V6O13 and synthesis of defect mixed-valence V0.92O2 rutile at high pressures and temperatures	260	FIRST FLOOR	95	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Hakanpää	Johanna	Jonca Dardeniz; Abdennour Zeboudin; Sami Khan; Neva Stucchi; Giulia Franceschin; Samah Al Khasoneh; Gianluca Iori	New access model at PETRA III & future PETRA IV beamline at DESY	332	FIRST FLOOR	57	27 August, Tue.	MS23 - Future of light sources and XFEL
Hans	Philipp		Enhanced Characterization of Ancient Glasses through Advanced Tomographic Techniques @ SESAME Synchrotron	120	THIRD FLOOR	118	29 August, Thur.	MS36
Haozhe Liu	Arthur		Phase diagram determination at high-pressure and low-temperature conditions	104	FIRST FLOOR	101	28 August, Wed.	MS27
Hari	Krishna		Biological piezoelectric materials as high-performance, eco-friendly structural health monitors	460	THIRD FLOOR	112	27 August, Tue.	MS28 - Structural characterization of Energy Harvesting and Conversion Materials
Havlickova	Petra	Anna Koutska; Ivana Kuta Smatanova; Michaela Fencikova	From Uncertainty to Molecular Mechanism: Missense Mutations in BRAF and MAP2K1 in Cognitive Disorders	665	GROUND FLOOR	15	28 August, Wed.	MS05
Heine	Andreas		Fragment-based inhibitor development to fight Shigellosis	509	GROUND FLOOR	11	28 August, Wed.	MS05
Heinemann	Udo	Qianqian Ming; Yvette Roske; Maria Rutkiewicz; Jianhui Wang	Structural and target DNA-binding studies of Grainyhead/CP2 transcription factors	595	GROUND FLOOR	7	29 August, Thur.	MS01
Henriques	Margarida		Incommensurate magnetic modulations of the 2D-layered Ho3Co described by superspace symmetry	425	FIRST FLOOR	86	28 August, Wed.	MS19
Hikita	Masahide		Current status of microspectroscopic systems for the macromolecular crystallography beamline AR-NW12A at the Photon Factory	578	GROUND FLOOR	6	28 August, Wed.	MS03
Hinuma	Yoyo		On the effectiveness of first-year-of-university math and somewhat brute force computing when developing new methods in crystallography	10	SECOND FLOOR	104	29 August, Thur.	MS38
Hinuma	Yoyo		Finding the Bravais lattice of a "1/N" size supercell from error-containing lattice parameters	361	FIRST FLOOR	52	29 August, Thur.	MS22
Ho	Feng-Hua		Structure Determinations and Phase Transition Study on New One-dimensional Fe(II) Coordination Polymers Using Tetrazole Derivatives	435	FIRST FLOOR	71	27 August, Tue.	MS33 - Correlate molecular structure with materials properties

FIRST AUTHOR'S LAST NAME	FIRST AUTHOR'S FIRST NAME	OTHER AUTHORS' NAMES	TITLE	POSTER ID	FLOOR	PANEL NR.	DAY	SESSION
Hofer	Gerhard		Protein serial electron diffraction for everyone	687	FIRST FLOOR	42	27 August, Tue.	MS15 - ED small waves, big ponds – Biomolecules and macromolecules
Holczbauer	Tamás		The effect of high pressure on organocatalyst containing crystal structures	641	FIRST FLOOR	89	29 August, Thur.	MS27
Hordichuk	Oleh		Hybrid materials of metal halide nano-sized clusters orderly confined in single crystal metal-organic reticular materials	570	FIRST FLOOR	77	29 August, Thur.	MS30
Hsu	I-Jui		Characterization of phase transition behaviors of iron complexes based on pyridyl-tetrazole ligands	436	THIRD FLOOR	107	29 August, Thur.	MS33
Hu	Junyi		A six-membered ring molecular sieve achieved by 3D-3D topotactic transformation	249	THIRD FLOOR	131	28 August, Wed.	MS30
Hu	Chengdao	Cameron J. G. Wilson; Simon Parsons	Centring of Diamond Anvil Cells Using an Optical Sensor	514	FIRST FLOOR	85	29 August, Thur.	MS27
Hulai	Natalia	John D. Chargo, Christopher W. Collins, Luke W. 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	455	FIRST FLOOR	69	28 August, Wed.	MS17
Hunter	Charlotte		EBNA1 PROTACs	85	FIRST FLOOR	39	28 August, Wed.	MS10
Ignatev	Vladislav	Paulina Dominiak	The influence of wave function's basis set on the fit of multipole model to wave function	28	FIRST FLOOR	45	28 August, Wed.	MS11
Ilkaeva	Marina		In situ PXRD studies of poly(heptazine imide)-based adsorbents	659	FIRST FLOOR	79	29 August, Thur.	MS30
Iqbal	Waseem		Efficient Nickel and Cobalt Recovery by Metal–Organic Framework based Mixed Matrix Membranes (MMM-MOFs)	517	FIRST FLOOR	75	29 August, Thur.	MS30
Irmer	Erhard		Crystal Structure Analysis in School	211	THIRD FLOOR	137	27 August, Tue.	MS41 - Approaches and tools for learning crystallography efficiently and avoiding misconceptions
Jacobs	Francois		In search of new interactions for rhenium metal-based pharmaceutical development.	41	FIRST FLOOR	36	28 August, Wed.	MS10
Jandl	Christian	Benjamin A. Palmer; Laura Samperisi	Electron diffraction for direct structural determination of biogenic crystals	523	GROUND FLOOR	22	29 August, Thur.	MS20
Jarzemska	Katarzyna		Nanosecond-lived excimer observation in a rhodium(I) crystalline complex via time-resolved Laue diffraction	131	FIRST FLOOR	65	27 August, Tue.	MS33 - Correlate molecular structure with materials properties
Jia	Xu	Chongting Ren; Luc VanMeervelt	Crystallographic insights into diverse water stability mechanisms of Zn-MOFs	386	THIRD FLOOR	135	28 August, Wed.	MS30
Jia	Xu	Luc VanMeervelt; Chongting Ren	Control of structure and interpenetration degree transformations in Zn-MOFs	389	FIRST FLOOR	72	29 August, Thur.	MS30
Johansen	Morten		Structural effects from varying the Fe/Mn ratio in layered NaFeyMn1-yO2 for Na-ion batteries	624	FIRST FLOOR	68	29 August, Thur.	MS25
John	Sanjay	Roland Resel	Identification of a metastable phase and an unstable phase in 1,1'- Binaphthalene	640	FIRST FLOOR	101	27 August, Tue.	MS26 - Chirality: Meeting point of crystallography, chemistry and topology
Jones	Andrew		X-ray diffraction for battery analysis	360	FIRST FLOOR	64	29 August, Thur.	MS25
Joseph	Boby		Hard X-ray Diffraction Beamlines at Elettra for Material Science : The Present and the Future	539	FIRST FLOOR	61	27 August, Tue.	MS23 - Future of light sources and XFEL
Jurić	Marijana	Ana Lozančić; Sanja Burazer; Sanja Renka; Krešimir Molčanov; Lidija Androš Dubraja	Structural, conductive and precursor properties of heterometallic compounds containing alkylammonium cations	446	THIRD FLOOR	108	29 August, Thur.	MS33
Kamale	Chinmay		Structure-guided improvement of glucose tolerance and catalytic efficiency of β -glucosidase from <i>Clostridium thermocellum</i> for industrial bioethanol production	314	GROUND FLOOR	18	28 August, Wed.	MS06
Kapetanaki	Sofia		Study of the conformational dynamics of a bacterial photoactivated adenylate cyclase	242	GROUND FLOOR	12	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature

FIRST AUTHOR'S LAST NAME	FIRST AUTHOR'S FIRST NAME	OTHER AUTHORS' NAMES	TITLE	POSTER ID	FLOOR	PANEL NR.	DAY	SESSION
Karimova	Oxana		High temperature single crystal X-ray diffraction of Pd bismuthides	565	FIRST FLOOR	87	29 August, Thur.	MS27
Karlsen	Martin Aaskov		Digging deeper into the irreversible disordering of nanocrystalline TiO ₂ -rutile electrodes	287	FIRST FLOOR	30	28 August, Wed.	MS35
Karothu	Durga Prasad		Exceptionally high work density of a ferroelectric dynamic organic crystal around room temperature	631	THIRD FLOOR	114	27 August, Tue.	MS28 - Structural characterization of Energy Harvesting and Conversion Materials
Kascakova	Barbora		Targeting 3Cpro: A Promising Approach for Inhibiting Enterovirus D68	653	FIRST FLOOR	34	29 August, Thur.	MS10
Kaszubowski	Oskar		Combining SC-XRD, micro-PXRD and 3D ED in the structural description of dehydration of nucleotides and nucleotide-based drug crystals	180	FIRST FLOOR	52	27 August, Tue.	MS20 - When can ED challenges XRD in small molecule crystallography?
Kaźmierczak	Michał		What we have learned about negative linear compressibility studying cocrystal of 1,2-bis(4-pyridyl)ethane and fumaric acid	199	THIRD FLOOR	107	28 August, Wed.	MS27
Kedari	Ashwini	ASHWINI KEDARI	Structural perspective into rabies virus neutralization	471	FIRST FLOOR	30	27 August, Tue.	MS5 - Infectious and Neglected diseases
Keene	Tony	Viktorija Mikaite	Rad(ical) Naphthalimide-Based Coordination Polymers	79	THIRD FLOOR	127	28 August, Wed.	MS30
Keil	Eleanor		Understanding Carbon Dioxide Uptake in ZIFs Via In-Situ Single Crystal Diffraction	135	FIRST FLOOR	58	29 August, Thur.	MS25
Kekez	Ivana		Mgy a novel metagenomic esterase as an excellent target for environment friendly degradation of polylactic acid	652	FIRST FLOOR	27	28 August, Wed.	MS06
Khachatryan	Hamlet	Conor Wild; Frank von Delft	DiffEMA: Diffusion-based generative network for protein model local quality assessment and auto-completion	630	GROUND FLOOR	23	27 August, Tue.	MS4 - AI, software developments and Machine learning applied to MX and CryoEM
Khadiev	Azat	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 $\text{[SmS]}_{1.19}\text{[TaS]}_2$ Nanotubes	424	FIRST FLOOR	85	28 August, Wed.	MS19
Kherfi	Hamza		Different Hydrogen-bond networks in two 1D bimetallic oxalate compounds: $\text{ACr(C}_2\text{O}_4)_2(\text{H}_2\text{O})_4$ (A = Li, Na)	26	SECOND FLOOR	105	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Kholina	Yevhenia	Arkadiy Simonov	Unconventional charge transfer transition in KCo[Fe] Prussian Blue Analogue	576	THIRD FLOOR	149	29 August, Thur.	MS29
Kim	Hye-Yeon		Structural and biophysical characterization of antigen-antibody complexes	442	FIRST FLOOR	29	27 August, Tue.	MS5 - Infectious and Neglected diseases
Kingsbury	Christopher J.		Molecular symmetry and art: visualizing the near-symmetry of molecules in Piet Mondrian's De Stijl	499	FIRST FLOOR	99	27 August, Tue.	MS26 - Chirality: Meeting point of crystallography, chemistry and topology
Kkrarcha	Hadda		Lattice constants prediction and thermochemistry of hexahalometallate A ₂ MX ₆	200	THIRD FLOOR	155	27 August, Tue.	MS29 - Structural characterization in Functional materials
Kleemiss	Florian		Machine guess of scattering factors - SALTED-NoSpherA2	318	FIRST FLOOR	51	28 August, Wed.	MS11
Kohli	Varun		Tuning LLM models to predict protein's 3D structure	431	GROUND FLOOR	19	27 August, Tue.	MS4 - AI, software developments and Machine learning applied to MX and CryoEM
Konovalova	Iryna		Application of quantum chemistry methods to analyse supramolecular architecture of halogen substituted anilines	700	FIRST FLOOR	87	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography
Kost	Niklas		Oxidation state of ultrasmall dodecylamine-coated palladium nanoparticles probed by X-ray techniques	283	THIRD FLOOR	115	28 August, Wed.	MS29
Koutska	Anna	Anna Koutska	Investigating the effect of neurodevelopmental disorder missense variants on cognitive function with Drosophila	664	GROUND FLOOR	14	28 August, Wed.	MS05
Kovalevskiy	Oleg		The next generation of AlphaFold: accelerating structural biology research	454	GROUND FLOOR	20	27 August, Tue.	MS4 - AI, software developments and Machine learning applied to MX and CryoEM

FIRST AUTHOR'S LAST NAME	FIRST AUTHOR'S FIRST NAME	OTHER AUTHORS' NAMES	TITLE	POSTER ID	FLOOR	PANEL NR.	DAY	SESSION
Kováts	Éva	Dávid Földes; Gábor Bortel; Sándor Pekker	A new chiral metal-organic framework with spiranes	563	FIRST FLOOR	76	29 August, Thur.	MS30
Krajnak	Matus	Gearóid Mangan	MerlinEM, the universal detector for 4D STEM and 3D ED	306	FIRST FLOOR	57	28 August, Wed.	MS16
Krause	Lennard		SINCRYS – single-crystal materials science beamline at MAX IV	371	FIRST FLOOR	58	27 August, Tue.	MS23 - Future of light sources and XFEL
Kraut	Daniel		Polar amalgams: structure-property relations in bad metals	284	FIRST FLOOR	97	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Kravets	Kateryna		Diversity of the host-guest crystalline assemblies of p-sulfonatocalix[n]arenes with benzamides	208	FIRST FLOOR	93	29 August, Thur.	MS31
Kremer	Marius		New developments in non-ambient X-ray diffraction instrumentation	440	FIRST FLOOR	96	28 August, Wed.	MS24
Krengel	Ute		New structural insights into bacterial colonization by <i>Vibrio cholerae</i>	508	GROUND FLOOR	10	28 August, Wed.	MS05
Krengel	Ute	Natalia Mojica	Structural basis for the differential toxicity of cholera toxin and heat-labile enterotoxin	597	GROUND FLOOR	13	28 August, Wed.	MS05
Kretić	Danijela	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.	623	THIRD FLOOR	113	29 August, Thur.	MS33
Krysiak	Yaşar		High temperature electron diffraction on organic crystals: in situ crystal structure determination of Pigment Orange 34	409	GROUND FLOOR	18	29 August, Thur.	MS20
Książek	Maria		Slow Thermally-Induced Spin Crossover in the Two-Dimensional Network [Fe(bbtr)3](BF4)2	227	THIRD FLOOR	109	28 August, Wed.	MS27
Kubicki	Maciej		Experimental electron density distribution in cocrystals of theophylline and pyromellitic acid	215	THIRD FLOOR	136	28 August, Wed.	MS32
Kumar	Anil		The charge density derived from electron diffraction on simulated data differs from that obtained from X-ray diffraction	70	FIRST FLOOR	43	27 August, Tue.	MS21 - Electron diffraction joining forces with quantum crystallography towards materials science applications
Kumar	Lavanya		Understanding the electronic structure of halogen bonding with heavy pnictogen acceptor atoms: Insights from charge density and DFT analysis	161	FIRST FLOOR	84	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography
Kurlin	Vitaliy	Daniel Widdowson	Ultra-fast detection of (near-)duplicate structures across major crystal databases	150	FIRST FLOOR	48	29 August, Thur.	MS22
Kurlin	Vitaliy		The Crystal Isometry Principle has made transparent the black boxes of structural databases	491	THIRD FLOOR	132	29 August, Thur.	MS39
Kusz	Joachim		X-ray diffraction study of bis(tetrazolyl)alkane-based Fe(II) coordination polymers	229	THIRD FLOOR	111	28 August, Wed.	MS29
Kuzel	Radomir		Growth of thin films of hexaferrites prepared by chemical solution deposition	693	THIRD FLOOR	155	29 August, Thur.	MS29
Kyazumov	Mahmud		New rotation electron-diffraction methods and their applications	31	FIRST FLOOR	54	28 August, Wed.	MS16
Lahey-Rudolph	Mia		Crystals in living insect cells: Of detection, serial diffraction and genuine co-factor discovery.	480	GROUND FLOOR	4	28 August, Wed.	MS03
Lamba	Doriano		Disenchanting the mechanism underlying the covalent methanesulfonyl fluoride acetylcholinesterase adduct formation and evolution: structural and mechanistic insights into an aged-like inactive complex susceptible to reactivation by a combination of	629	FIRST FLOOR	25	28 August, Wed.	MS06
Lampronti	Giulio Isacco		The scientific case for in-situ diffraction investigations of mechanochemical processes: recent developments and state of the art.	489	FIRST FLOOR	65	29 August, Thur.	MS25
Lanza	Arianna		Anion-mediated solid-state polymerization of a simple Cu-bpy complex, investigated via electron diffraction	662	THIRD FLOOR	151	29 August, Thur.	MS29

FIRST AUTHOR'S LAST NAME	FIRST AUTHOR'S FIRST NAME	OTHER AUTHORS' NAMES	TITLE	POSTER ID	FLOOR	PANEL NR.	DAY	SESSION
Lazarova	Hristina		Grace titanium silicate-1 for treatment of Crystal violet and Methylene blue by wastewater	606	FIRST FLOOR	78	29 August, Thur.	MS30
Lazzari	Rémi		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)	241	FIRST FLOOR	59	29 August, Thur.	MS25
Le Garff	Paul		Supramolecular isomerism in coordination polymers of Cd(II) with an imidazole based dipodal ligand	274	THIRD FLOOR	138	28 August, Wed.	MS32
Leubner	Nathan		In-situ characterization of the epitaxial growth of BaTiO ₃ thin films by pulsed laser deposition using synchrotron radiation	289	FIRST FLOOR	61	29 August, Thur.	MS25
Levendis	Demetrius		Crystallographic study of NaClO ₃ and NaBrO ₃ : addressing misconceptions about chirality, absolute configuration, and optical rotation	24	FIRST FLOOR	98	27 August, Tue.	MS26 - Chirality: Meeting point of crystallography, chemistry and topology
Li	Zhao		In situ synchrotron-based grazing incidence X-ray diffraction study on the solid-liquid interface of graphene oxide	617	FIRST FLOOR	67	29 August, Thur.	MS25
Liermann	H.-P.		Status and new developments at the Extreme Conditions beamline (ECB, P02.2) PETRA III, DESY	692	FIRST FLOOR	91	29 August, Thur.	MS27
Lima	Gustavo Jones		Crystal Structure, Hirshfeld Surface Analysis and Spectroscopic Studies of Newly Synthesized Dithiocarbamate Pyrazole Compound	688	FIRST FLOOR	102	29 August, Thur.	MS31
Lin	Hong-Cheu		Force-triggered optical-type and nonometric mechanofluorescence of Polyethylene Elastomers Containing Innovatively Modified [c2] Daisy Chain Molecules with Promoted Stretchabilities and Toughnesses	502	THIRD FLOOR	146	29 August, Thur.	MS29
Lissner	Falk	Thomas Schleid; Kurt Walenta	The Trigonal Crystal Structure of Matildite-Type AgBiS ₂ Revisited	470	FIRST FLOOR	74	28 August, Wed.	MS17
Liu	Jie		Investigation of A Novel Organocobalt Complex of B12 Model Catalyst	326	THIRD FLOOR	119	28 August, Wed.	MS29
Locke	Ralf Jules Christian	Thomas Schleid	Closing Some Gaps of Knowledge: Single Crystals of Nd ₂ [Sb ₄ O ₈]Cl ₂	468	FIRST FLOOR	72	28 August, Wed.	MS17
Locke	Ralf Jules Christian	Thomas Schleid	Pr ₃ O[AsO ₃] ₂ : The First Oxide Iodide Oxoarsenate of the Rare-Earth Metals	469	FIRST FLOOR	73	28 August, Wed.	MS17
Longcake	Alexandra		Crystallising natural products via high-throughput nanodroplet crystallisation protocols.	195	GROUND FLOOR	10	29 August, Thur.	MS08
Losus	Renny Louis Anto Maria		Conformational diversity of tetra-O-ethyl-p-tert-butylcalix[4]arene and its molecular dynamics in the single-crystal unity	175	THIRD FLOOR	122	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Lübben	Anna		Leveraging Deep Learning for smart sample alignment	545	GROUND FLOOR	21	27 August, Tue.	MS4 - AI, software developments and Machine learning applied to MX and CryoEM
Lucchini	Davide		Crystal structures of rhenium(V) complexes with thiosemicarbazonate ligands	715	FIRST FLOOR	44	28 August, Wed.	MS10
Luhong-Wang Liu	Lisa		Pressure induced transitions in two types of engineering oxides	113	FIRST FLOOR	102	28 August, Wed.	MS27
Luneau	Dominique		Electron diffraction boosts research on molecule-based magnets	571	FIRST FLOOR	89	28 August, Wed.	MS19
Lutz	Martin		Pseudo-centrosymmetry can confuse automatic space group determination	16	THIRD FLOOR	127	29 August, Thur.	MS39
Macetti	Giovanni		Symmetry-constrained Monte Carlo for crystal structure prediction	160	THIRD FLOOR	121	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Madura	Izabela		Crystalline forms of vitamin B7 - an example of a crystal engineer's nightmare	322	THIRD FLOOR	140	28 August, Wed.	MS32

FIRST AUTHOR'S LAST NAME	FIRST AUTHOR'S FIRST NAME	OTHER AUTHORS' NAMES	TITLE	POSTER ID	FLOOR	PANEL NR.	DAY	SESSION
Malenov	Dušan		Coordinated water as hydrogen bond acceptor – a joint CSD and DFT perspective	374	FIRST FLOOR	97	29 August, Thur.	MS31
Malinska	Maura		Decoding Amino Acid@Cucurbit[7]uril through X-ray diffraction: Balancing Hydrophobicity and Ion-Dipole Interactions	258	FIRST FLOOR	94	29 August, Thur.	MS31
Maloney	Andrew G. P.		Correlating particle informatics with surface wetting measurements	393	FIRST FLOOR	69	27 August, Tue.	MS33 - Correlate molecular structure with materials properties
Maly	Martin		Work with serial crystallography data from CrystFEL and xia2.sxx in CCP4 suite	128	GROUND FLOOR	7	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
Managutti	Praveen		Enhancing SOFC Anode Performance through Cerium and Nickel Doping in PrBaMn2O5+δ Structures	683	FIRST FLOOR	71	29 August, Thur.	MS25
Marchetti	Daniilo	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	81	FIRST FLOOR	51	27 August, Tue.	MS20 - When can ED challenges XRD in small molecule crystallography?
Marek	Martin		Structural basis for NanoLuc luciferase action	231	GROUND FLOOR	3	27 August, Tue.	MS02 - Hot structures
Marshall	George		Order-disorder control in functional oxides	152	THIRD FLOOR	154	27 August, Tue.	MS29 - Structural characterization in Functional materials
Matković-Čalogović	Dubravka	Ivica Đilović	Robustness and stability of the L-carnosine copper(II) dimer. Coordinatively unsaturated sites of the high-temperature structure	673	THIRD FLOOR	116	29 August, Thur.	MS33
Mauri	Anna		Unveiling the crystallochemistry of a soft covalent organic framework during benzene and cyclohexane adsorption by in situ powder X-ray diffraction	119	THIRD FLOOR	128	28 August, Wed.	MS30
May	Nóra		Solid and solution state structures of Cu(II) – macrochelates developed for theranostic purposes	324	THIRD FLOOR	118	28 August, Wed.	MS29
May	Zoltán		Portable handheld XRF and μ -XRD examination of a late Roman copper cauldron	697	THIRD FLOOR	123	29 August, Thur.	MS36
Mazzeo	Paolo P.		On the Mechanism of Cocrystal Formation by Mechanochemical Reaction via Low Melting Eutectic: A Time-Resolved In Situ Monitoring Investigation	547	FIRST FLOOR	101	29 August, Thur.	MS31
McDonagh	David		Predicting Protein Crystal Solvent Content with Machine Learning	222	FIRST FLOOR	50	29 August, Thur.	MS22
McPherson	James	James McPherson	Metal-organic frameworks with zero-valent metal nodes	441	GROUND FLOOR	19	29 August, Thur.	MS20
Merkys	Andrius		Quality control of the chemical information in the Crystallography Open Database	497	THIRD FLOOR	133	29 August, Thur.	MS39
Merlini	Marco		The effect of iron on high-pressure behavior and phase transition in srebrodolskite-brownmillerite (CaFeO _{2.5} -CaAlO _{2.5})	427	FIRST FLOOR	48	27 August, Tue.	MS18 - Crystal-chemistry of minerals in the Universe: genesis, phase stability, and planetological implications
Miletich	Ronald		Disordered rhombohedral K ₂ Ca ₂ (CO ₃) ₃ : a supposedly transient state within an ambiguous transformation route on decompression	245	FIRST FLOOR	93	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Miloš	Sofija		Crystallography of the pressure-induced structural phase transitions in K ₂ Ca(CO ₃) ₂ and K ₂ Ca ₂ (CO ₃) ₃ carbonates	235	FIRST FLOOR	92	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Moeck	Peter		Symmetries and pseudo-symmetries in a sophisticated piece of graphic art and beyond	13	THIRD FLOOR	117	29 August, Thur.	MS36
Mokolokolo	Pennie		Rhodium(I) Carbonyl Complexes as Model Nano-Wired Assemblies	95	FIRST FLOOR	64	27 August, Tue.	MS33 - Correlate molecular structure with materials properties
Molčanov	Krešimir		Extended motives of two-electron multicentre bonds (pancake bonds): from discrete dimers to 2D networks	50	FIRST FLOOR	81	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography

FIRST AUTHOR'S LAST NAME	FIRST AUTHOR'S FIRST NAME	OTHER AUTHORS' NAMES	TITLE	POSTER ID	FLOOR	PANEL NR.	DAY	SESSION
Molčanov	Lidija	Krešimir Molčanov; Marijana Jurić; Luka Pavić	Charge transfer causes bulk conductivity through π -hole interactions	90	THIRD FLOOR	128	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Moncol	Jan		Crystal structure of new palladium(II) salicylate complexes with N,N-donor ligands	704	FIRST FLOOR	88	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography
Montebault	Clément		Degradation processes of colored papyri from Ancient Egypt	145	THIRD FLOOR	120	29 August, Thur.	MS36
Morana	Marta	Arianna Minelli; Alexei Bosak; Luca Bindi; Giovanni Orazio Lepore	Temperature dependence of single-crystal diffuse scattering in cupropearceite, [Cu ₆ As ₂ S ₇][Ag ₉ Cu ₅ S ₄]	366	FIRST FLOOR	67	28 August, Wed.	MS17
Moroni	Marco		Rationalizing the chiroptical behaviour of chiral hybrid metal halides: the role of composition and crystal structure	290	THIRD FLOOR	116	28 August, Wed.	MS29
Moszczyńska	Ida		Competition between CH \cdots π and CH \cdots M contacts in metallocenes structures	226	THIRD FLOOR	108	28 August, Wed.	MS27
Motaln	Klemen	Kshitij Gurung; Petr Brázda; Lukáš Palatinus; Matic Lozinšek	Structural investigation of fluoridopalladates(IV) by 3D ED	637	GROUND FLOOR	23	29 August, Thur.	MS20
Mugnaioli	Enrico		A combination of X-ray and electron crystallographic methods for understanding the origin of sector-zoning birefringent garnets with almandine-grossular composition	217	FIRST FLOOR	82	28 August, Wed.	MS19
Naumkina	Yelizaveta		Characterization of Apremilast – halogen benzoic acids cocrystals	252	THIRD FLOOR	137	28 August, Wed.	MS32
Neels	Antonia		Complex nanoparticle systems in motion: a holistic analytical approach for dynamical studies in biological environments	555	FIRST FLOOR	66	29 August, Thur.	MS25
Nemčovičová	Ivana		Small glycomimetic serves as antagonist to viral glycoprotein HCMV UL141 to inhibit the TRAIL death receptor binding	178	FIRST FLOOR	43	28 August, Wed.	MS10
Nemec	Ivan		Interplay of Halogen Bonding and Semi-Coordination in Co(II) Single-Ion Magnets	5	SECOND FLOOR	104	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Nénerť	Gwilherm		In-situ investigation of water harvesting by CAU-10-OH metal organic framework: a 2-steps process	336	THIRD FLOOR	133	28 August, Wed.	MS30
Novelli	Giulia		Investigating Pharmaceutical Solid Forms at High Pressure	167	SECOND FLOOR	106	28 August, Wed.	MS27
Nusser	Lukas		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	321	FIRST FLOOR	77	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Oeckler	Oliver	Paul Sicher	Fe-based skutterudite-like compounds	308	THIRD FLOOR	109	27 August, Tue.	MS28 - Structural characterization of Energy Harvesting and Conversion Materials
Oeffner	Robert		A Joint X-ray/cryo-EM platform for fragment-based drug discovery	698	FIRST FLOOR	56	29 August, Thur.	MS22
Oksanen	Esko		Neutron structure of Leishmania mexicana triosephosphate isomerase variant E97Q reveals a possible general acid	357	GROUND FLOOR	19	28 August, Wed.	MS06
Orr	Christian		Spherical Crystals: Laser Shaping of Biological and Chemical Materials	453	FIRST FLOOR	60	27 August, Tue.	MS23 - Future of light sources and XFEL
Ors	Taylan	Irena Déroche; Jean-Louis Paillaud	Localization of Na ⁺ cations within nanozeolite ECR-1 using a 3D ED method	261	FIRST FLOOR	83	28 August, Wed.	MS19
Otteny	Markus		From Laves to Zintl: AlI(Mg _{1-x} In _x) ₂ compounds (AlI=Ca, Sr, Ba)	342	FIRST FLOOR	79	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Ouali	Naima		Residual stresses determination and analysis in dissimilar rotary friction joints using X-ray diffraction method	292	THIRD FLOOR	117	28 August, Wed.	MS29
Palerma	Marta		Crystal structures of human histone deacetylase 8 in complex with novel hydroxamic acid inhibitors	372	FIRST FLOOR	27	29 August, Thur.	MS10

FIRST AUTHOR'S LAST NAME	FIRST AUTHOR'S FIRST NAME	OTHER AUTHORS' NAMES	TITLE	POSTER ID	FLOOR	PANEL NR.	DAY	SESSION
Parisi	Emmanuele		Controlling particle properties via crystal engineering: an example on quercetin hydrates, solvates and cocrystals.	593	THIRD FLOOR	142	28 August, Wed.	MS32
Park	SoHyun		Second-harmonic generation effect enhanced by Li+ substitution for Na+ in (Li _x Na _{6-x})Mo ₉ O ₃₀	395	THIRD FLOOR	122	28 August, Wed.	MS29
Patil	Sanket	Parijat Das; Dilip Badgajar; Prasenjit Bhaumik	Structural and functional analysis of a pore forming toxin from Streptococcus mitis	246	GROUND FLOOR	13	29 August, Thur.	MS09
Pavlyuk	Nazar	Volodymyr Pavlyuk; Helmut Ehrenberg; Grygory Dmytriv	Crystal structure and hydrogenation properties of the Mg ₆ CoSn ternary compound	333	THIRD FLOOR	111	27 August, Tue.	MS28 - Structural characterization of Energy Harvesting and Conversion Materials
Percoco	Rita Maria		Novel BioMOF@PAN Mixed Matrix Membranes as Highly Per-formant Adsorbing Materials for Multiple Heavy Metal Ions Removal	516	FIRST FLOOR	74	29 August, Thur.	MS30
Perles	Josefina		Mn(II) organo-inorganic salts as stimulus-responsive luminescent compounds	546	THIRD FLOOR	109	29 August, Thur.	MS33
Petrovic	Marko	David McDonagh; David Waterman	Automating the 3DED/MicroED data processing at Diamond Light Source's Electron Bio-Imaging Centre	42	FIRST FLOOR	45	29 August, Thur.	MS22
Pfanzagl	Vera		Myeloperoxidase dimerization in solution is mediated by interface glycans	562	GROUND FLOOR	23	28 August, Wed.	MS06
Pietrzak	Anna		Unraveling the mysteries of intramolecular hydrogen bonding defined by the phosphoryl group	205	FIRST FLOOR	92	29 August, Thur.	MS31
Pindelska	Edyta		New multicomponent systems of the anti-cancer drug erlotynib	607	THIRD FLOOR	143	28 August, Wed.	MS32
Pompidor	Guillaume		High throughput fragment screening at the beamline P11 at PETRA III	275	FIRST FLOOR	25	29 August, Thur.	MS10
Pong	Way-Faung		Coupling between spin and lattice in an XY-like spin-glass (Ni _{0.40} Mn _{0.60})TiO ₃	103	FIRST FLOOR	83	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography
Posavec	Lidija		Ternary halogen-bonded cocrystal design using Ni(II) complex containing isothiocyanate ligands as halogen bond acceptor species	66	THIRD FLOOR	125	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Potempa	Kinga		Insights into role of non-covalent interactions in achieving pressure-induced linkage isomerism of nitrite ligand.	72	THIRD FLOOR	126	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Privitera	Mario		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	157	FIRST FLOOR	42	28 August, Wed.	MS10
Psycharis	Vassilis		Structure relations of belite and alite polymorphs	552	FIRST FLOOR	78	28 August, Wed.	MS17
Putra	Okky		Unveiling dehydration and solid-solid phase transition through single crystal-to-single crystal transformation: A case study of AZD9898	661	THIRD FLOOR	140	29 August, Thur.	MS40
Qi	Ji		Correlation between structure and dynamic properties in SCO complex Fe(PM-BIA) ₂ (NCS) ₂	560	THIRD FLOOR	148	29 August, Thur.	MS29
Radanović	Mirjana		Crystal structure of a copper(I) complex with the Schiff base of 2-(diphenylphosphino)benzaldehyde and aminoguanidine	420	THIRD FLOOR	125	28 August, Wed.	MS29
Radovanović	Lidija		Crystallographic and quantum chemical studies of xanthen-1,8(2H)-dione derivatives	30	THIRD FLOOR	142	27 August, Tue.	MS29 - Structural characterization in Functional materials
Rainer	Daniel N.		Complementing XRD at the national level – 3DED and the UK National Electron Diffraction Facility (NEDF)	237	FIRST FLOOR	54	27 August, Tue.	MS20 - When can ED challenges XRD in small molecule crystallography?
Raptopoulou	Catherine		Chiral heterometallic Cu/Ln complexes from enantiopure Schiff base ligands	608	FIRST FLOOR	100	27 August, Tue.	MS26 - Chirality: Meeting point of crystallography, chemistry and topology
Ratajczyk	Paulina	Michał Andrzejewski; Andrzej Katrusiak; Lucia Maini; Marianna Marchini; Francesco Marin; Szymon Sobczak	Pressure- and temperature-driven polymorphism in PDI-C6	156	SECOND FLOOR	105	28 August, Wed.	MS27

FIRST AUTHOR'S LAST NAME	FIRST AUTHOR'S FIRST NAME	OTHER AUTHORS' NAMES	TITLE	POSTER ID	FLOOR	PANEL NR.	DAY	SESSION
Ratcliff	William	Satvik Lolla; Haotong Liang; Aaron Kusne; Ichiro Takeuchi	Semi and self supervised approaches to space group and Bravais lattice determination	186	FIRST FLOOR	49	29 August, Thur.	MS22
Raza	Arsez		Experimental demonstration of a second polymorph of Osmium acetylacetonate(III) by magnetometric technique.	666	FIRST FLOOR	90	28 August, Wed.	MS19
Rečko	Katarzyna	Marta Orzechowska; Maria Biernacka; Beata Kalska-Szostko	Magnetism of gallium cuboferrites	584	THIRD FLOOR	150	29 August, Thur.	MS29
Rekis	Toms		Testing "PhAI" for solving crystal structures from electron diffraction and powder X-ray diffraction data	388	FIRST FLOOR	58	28 August, Wed.	MS16
Reubold	Thomas		Crystal structure of the effector/metaeffector pair SidL/LegA11 from Legionella pneumophila	667	GROUND FLOOR	16	28 August, Wed.	MS05
Ribaldone	Chiara		Combining Molecular Dynamics Simulations with Topological Analysis of the Bonding in Crystalline Systems	574	FIRST FLOOR	86	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography
Richert	Clemens		Second Generation Chaperones Support Cocrystallization of Long Flexible Chain Molecules	276	THIRD FLOOR	139	28 August, Wed.	MS32
Rodić	Marko	Milan Nešić; Matic Lozinšek; Niko Radulović	Insight into α -iminoamides: Hirshfeld atom refinement and evaluation of intermolecular interaction energies	83	FIRST FLOOR	47	28 August, Wed.	MS11
Rogan	Jelena		Crystal structure and computational study of cobalt(II) coordination polymer with 2,2'-dipyridylamine and anion of isophthalic acid	29	THIRD FLOOR	141	27 August, Tue.	MS29 - Structural characterization in Functional materials
Röhr	Caroline		Ca(Zn _{1-x} Cd _x) ₃ /5: Disorder models for known and new hexagonal intermetallics	669	FIRST FLOOR	44	29 August, Thur.	MS14
Rosa	Patrick		Molecular ceramics of spin crossover materials by Cool-SPS for barocaloric refrigeration	522	FIRST FLOOR	86	29 August, Thur.	MS27
Rouag	Raounek		Synthesis, crystal structure, biological properties and theoretical calculations of 2-(2-aminophenyl)-1H-benzimidazol-3-ium dichloride	140	THIRD FLOOR	151	27 August, Tue.	MS29 - Structural characterization in Functional materials
Round	Adam		The SPB/SFX instrument at the European XFEL - capabilities and scientific use cases for room temperature dynamics.	385	GROUND FLOOR	1	28 August, Wed.	MS03
Round	Ekaterina		Integrated sample preparation, characterization and delivery for room temperature serial crystallography at the European XFEL	551	GROUND FLOOR	5	28 August, Wed.	MS03
Rouquette	Jerome		BaCo ₂ with Tetrahedral Cobalt Coordination: Unlocking Energy Storage and Conversion in BaCo _{2-δ} Materials	645	FIRST FLOOR	70	29 August, Thur.	MS25
Ruth	Paul Niklas		QCrBox: Unlocking (Quantum) Crystallography	696	FIRST FLOOR	52	28 August, Wed.	MS11
Rybicka	Paulina Maria		The effect of (not) applying symmetry constraints during refinement and using different local coordinate systems on local symmetry of atoms and atom types in the MATTS data bank	69	FIRST FLOOR	46	28 August, Wed.	MS11
Rzepka	Przemyslaw		Determining Active Sites in Zeolite Structures Using Anomalous Diffraction at the Al K-edge	474	FIRST FLOOR	73	29 August, Thur.	MS30
Sacharczuk	Natalia	Anna Olejniczak; Maciej Bujak; Marcin Podsiadlo	Molecular aggregations in crystals of butene isomers determined at high-pressure	127	FIRST FLOOR	103	28 August, Wed.	MS27
Sanchez Rodriguez	Filomeno		Moorhen: interactive model building on the web	59	GROUND FLOOR	15	27 August, Tue.	MS4 - AI, software developments and Machine learning applied to MX and CryoEM
Sangster	Calum	Fabio Nudelman	Use of 3D-ED as a Tool for Studying Mechanism of Formation of Complex Materials	495	GROUND FLOOR	21	29 August, Thur.	MS20
Santucci	Marco		PyFast-ADT: python-driven 3DED data collection and automatic crystal tracking	394	FIRST FLOOR	60	28 August, Wed.	MS16
Saric	Lovro	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	512	FIRST FLOOR	77	28 August, Wed.	MS17

FIRST AUTHOR'S LAST NAME	FIRST AUTHOR'S FIRST NAME	OTHER AUTHORS' NAMES	TITLE	POSTER ID	FLOOR	PANEL NR.	DAY	SESSION
Saridakis	Emmanuel		Protein thermodynamic properties, crystallisation, and the Hofmeister Series	572	GROUND FLOOR	11	29 August, Thur.	MS08
Satheasuweatha Marimuthu	Nirmala Devi		High-Pressure Structural Investigations of AuSn4 and its Potential Chemical Pressure Equivalent PtSn4	75	FIRST FLOOR	99	28 August, Wed.	MS27
Scatena	Rebecca		Hybrid improper ferroelectricity in columnar (NaY)MnMnTi4O12	488	THIRD FLOOR	145	29 August, Thur.	MS29
Scatena	Rebecca		The materials and magnetism beamline, I16 at diamond light source Ltd	678	FIRST FLOOR	91	28 August, Wed.	MS19
Schirò	Giorgio		Structural dynamics of a B12-dependent photoreceptor	601	GROUND FLOOR	7	28 August, Wed.	MS03
Schleid	Thomas	Felix Christian Goerigk	Gd2F[CO3][AsO3]: A Serendipitously Formed Gadolinium Fluoride Oxocarbonate Oxoarsenate(III)	467	FIRST FLOOR	71	28 August, Wed.	MS17
Schleissner	Pamela		From Protein Dynamics to Biological Function: The Impact of LCLS-II and the Center for Structural Dynamics in Biology	695	FIRST FLOOR	62	27 August, Tue.	MS23 - Future of light sources and XFEL
Schmidt	Ashley		Squeezing the most out of your high pressure data	423	FIRST FLOOR	83	29 August, Thur.	MS27
Schmitt	Yann		Challenging shortcomings in the field of 3D ED: a new cross-platform solution for various experimental set-ups	412	FIRST FLOOR	62	28 August, Wed.	MS16
Schulze	Manuel		A previously unnoticed RE-TM-antimonide: CeFeSb3.	331	THIRD FLOOR	120	28 August, Wed.	MS29
Selsabil Yeddiou	Belkis		Synthesis, crystal structure, Hirshfeld surface analysis and framework Energy study of a new Ni-Coordination complex with 1,10-phenanthroline	92	THIRD FLOOR	129	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Semjonova	Aina		Diversity and Similarity in Isonicotinamide Two-Component Phases with Alkyl Carboxylic Acids: Focus on Solvates	57	THIRD FLOOR	117	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Serrão	Guilherme		Quinolines as optimal Halogen-Bonding acceptors	450	FIRST FLOOR	100	29 August, Thur.	MS31
Setshedi	Itumeleng		Supramolecular synthesis, crystallization, and co-crystallization of combination drugs for the inhibition of mycobacteria species	125	FIRST FLOOR	25	27 August, Tue.	MS5 - Infectious and Neglected diseases
Shaw Stewart	Patrick		Sample preparation for routine and advanced structural biology ECM	14	GROUND FLOOR	5	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
Siebert	Alistair		HeXI: The High-energy Electron Xtallography Instrument at Diamond Light Source	21	FIRST FLOOR	53	28 August, Wed.	MS16
Simbrunner	Josef		Searching for new polymorphs by epitaxial growth	132	THIRD FLOOR	149	28 August, Wed.	MS40
Singh	Charandeep	Krishan Gopal Thakur	Structural insights into Polymorphic toxin –Immunity pair system of Bacillus subtilis	7	GROUND FLOOR	1	27 August, Tue.	MS02 - Hot structures
Sironi	Luca	Luca Sironi	Pre-nucleation clusters in liquid benzoic acid	159	THIRD FLOOR	131	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Sitshwele	Nazo		Influencing the reaction pathway in solid-state Diels-Alder cycloaddition using a vinyl substituent	137	GROUND FLOOR	8	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
Slawinski	Wojciech		BIG BOX modelling of Pair Distribution Function using RMCPProfile7 program	618	FIRST FLOOR	32	28 August, Wed.	MS35
Ślepokura	Katarzyna		Structural description of dehydration and polymerization in cGMP crystals in light of the origins of life.	410	THIRD FLOOR	135	29 August, Thur.	MS40
Śmietanińska-Nowak	Joanna		Application of advanced multidimensional analysis methods to study modulated structures of the Hyp-1/ANS protein complex	646	FIRST FLOOR	43	29 August, Thur.	MS14

FIRST AUTHOR'S LAST NAME	FIRST AUTHOR'S FIRST NAME	OTHER AUTHORS' NAMES	TITLE	POSTER ID	FLOOR	PANEL NR.	DAY	SESSION
Smith	Mark		The influence of reaction conditions on co-crystals of isoniazid derivatives	126	THIRD FLOOR	120	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Sobral Carvalho	Ana Carina		New hydrated salts of Sparfloxacin: a supramolecular synthon analysis	672	THIRD FLOOR	146	28 August, Wed.	MS32
Solokha	Pavlo		Long period stacking ordered (LPSO) Y-Ni-Mg phases studied by 3D electron diffraction	398	FIRST FLOOR	38	29 August, Thur.	MS14
Squeglia	Flavia	Valeria Napolitano	Crystallographic and functional studies of Kp-Iin, a nano-sized protective cage from <i>Klebsiella pneumoniae</i>	642	FIRST FLOOR	31	29 August, Thur.	MS10
Stanić	Petra		The role of multicentric pancake bond in 2D arrays of TCNQ radicals in crystals	44	FIRST FLOOR	80	27 August, Tue.	MS13 - Molecular structure and chemical bonding in the view of quantum crystallography
Strzalka	Radoslaw		The real space approach to the atomic structure of Tsai-type quasicrystal	558	FIRST FLOOR	40	29 August, Thur.	MS14
Stubbs	Jack		Droplet microfluidics for uniform microcrystallization and rapid mixing	154	GROUND FLOOR	9	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
Stürzer	Tobias		Masterful sample grilling starts here	475	FIRST FLOOR	75	28 August, Wed.	MS17
Sudol	Abigail		Extensive substrate recognition by streptococcal antibody-degrading enzymes	151	GROUND FLOOR	2	27 August, Tue.	MS02 - Hot structures
Suescun	Leopoldo		The search for the 4th stable polymorph of Lapachol	230	THIRD FLOOR	152	28 August, Wed.	MS40
Suh	Jeong-Yong		Structure-based design and optimization of fungal lipases to improve substrate binding and enzyme activity	244	FIRST FLOOR	40	27 August, Tue.	MS6 - Structural studies in Enzymology
Sun	Yuh-Ju	Chen-Hsi Chu; Min-Guan Lin; Chwan-Deng Hsiao	Insights into the molecular mechanism of ParABS system in chromosome partition by HpParA and HpParB	434	GROUND FLOOR	6	29 August, Thur.	MS01
Suryawanshi	Abhishek		Multiple high-resolution structures providing the insights of glucose tolerance in GH1 family β -glucosidases	111	FIRST FLOOR	38	27 August, Tue.	MS6 - Structural studies in Enzymology
Sutula	Szymon		Too small for XRD but perfectly sized for ED	298	FIRST FLOOR	55	27 August, Tue.	MS20 - When can ED challenges XRD in small molecule crystallography?
Suwinska	Kinga		Macrocyclic molecules as potential drugs carriers	302	FIRST FLOOR	96	29 August, Thur.	MS31
Szymański	Bartosz		Shedding a new light on nitro compounds: NIR-emitting quadrupole-structured dyes	68	THIRD FLOOR	145	27 August, Tue.	MS29 - Structural characterization in Functional materials
Szymon Sobczak		Szymon Sobczak	Piezosolvatochromic insights into solvent-solute interactions	130	THIRD FLOOR	130	27 August, Tue.	MS31 - Noncovalent interactions in structure design
Tailleur	Elodie		A multipurpose diffractometer for advanced SC-XRD experiments under T, P, E and hv	313	FIRST FLOOR	62	29 August, Thur.	MS25
Tarantino	Serena Chiara		A crystallographic approach to the study of dinosaur eggshells of 70 Ma from Mexico	532	THIRD FLOOR	121	29 August, Thur.	MS36
Tedesco	Consiglia		The peptoid's path to understand the role of CH \cdots OC and CO \cdots CO interactions in proteins	429	FIRST FLOOR	99	29 August, Thur.	MS31
Théron	Coline		X-ray powder diffraction: a hub in the integrative study of the schematic Holocene rock art	124	THIRD FLOOR	119	29 August, Thur.	MS36
Thompson	Sam		Chiral substitutions for promoting polar materials discovery	101	THIRD FLOOR	148	27 August, Tue.	MS29 - Structural characterization in Functional materials
Thompson	Paul		Design, Implementation, and Performance of Operando Anomalous Powder X-ray Diffraction (AXRD) Interleaved with X-ray Absorption Spectroscopy (XAS) Using a Scanning 2D Imaging Detector at the XMa5 Beamline	478	FIRST FLOOR	97	28 August, Wed.	MS24

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Tiberi	Michele		NF-Y acts as a molecular platform to guide the binding of the ER stress response factor to the ER-stress elements ERSE and ERSE II. A case of molecular "asymmetric symmetry"	408	GROUND FLOOR	5	29 August, Thur.	MS01
Tiwari	Bhaskar		Polymorphism of ribavirin at high pressure	451	THIRD FLOOR	136	29 August, Thur.	MS40
Többsens	Daniel M.		Deep insights into energy materials utilizing anomalous X-ray diffraction	181	THIRD FLOOR	108	27 August, Tue.	MS28 - Structural characterization of Energy Harvesting and Conversion Materials
Todorovic	Nikolina		Structure-based IgE-epitope investigation of the major cat allergen Fel d 4	225	FIRST FLOOR	26	27 August, Tue.	MS5 - Infectious and Neglected diseases
Toms	Tom		Incommensurate displacive and occupational modulation in the structures of [FexCr1-x(urea)6](NO3)3 (x = [0, 1]) complexes	325	FIRST FLOOR	36	29 August, Thur.	MS14
Tragheim	Ben		Competition between G-type, C-type and CE-type orbital ordering modes in Na- and Ca-doped Hg-quadruple manganite perovskites	35	THIRD FLOOR	143	27 August, Tue.	MS29 - Structural characterization in Functional materials
Uribe Rincon	Carla Margarita		Structural and spectroscopic characterisation of schafarzikite-type PbSbMO4 (M = Cr, Fe, Mn)	281	FIRST FLOOR	96	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Urzhumtsev	Alexandre		Direct real-space determination of atomic parameters from inhomogeneous cryoEM and crystallographic maps	164	GROUND FLOOR	16	27 August, Tue.	MS4 - AI, software developments and Machine learning applied to MX and CryoEM
Uski	Ville	Ville Uski	Introducing the next major release of CCP4: What's new?	598	GROUND FLOOR	22	27 August, Tue.	MS4 - AI, software developments and Machine learning applied to MX and CryoEM
Vaitkus	Antanas		Lost in translation – using CIF dictionaries for semantic data validation	496	THIRD FLOOR	125	29 August, Thur.	MS38
van Staden	Christo		In "Au" Over Metallophilic Interactions	56	SECOND FLOOR	106	27 August, Tue.	MS31 - Noncovalent interactions in structure design
van Terwingen	Steven		Tailoring halogen bond donors for crystal engineering	84	THIRD FLOOR	118	27 August, Tue.	MS32 - Advanced materials design with (co)crystal engineering: synthesis, crystal growth, structure and function
Vascon	Filippo	Matteo Bersani; Eleonora Gianquinto; Alice Legru; Federica Verdiora; Laurent Gava; 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	569	GROUND FLOOR	12	28 August, Wed.	MS05
Vijayakumar Syamala	Vishnu		Metallophilicity-assisted piezochromism in a Rh(I) complex: structural, energetic, electronic and spectroscopic investigations under pressure	87	FIRST FLOOR	100	28 August, Wed.	MS27
Virovets	Alexandr		Single-crystal XRD: Black box vs experienced crystallographer	320	THIRD FLOOR	130	29 August, Thur.	MS39
Vypriiskaia	Angelina		Neural Network-Assisted Crystal Detection for Automated Electron Diffraction Data Collection	466	FIRST FLOOR	63	28 August, Wed.	MS16
Wang	Gang		Topological crystalline insulator candidate ErAsS with hourglass fermion and magnetic-tuned topological phase transition	507	THIRD FLOOR	113	27 August, Tue.	MS28 - Structural characterization of Energy Harvesting and Conversion Materials
Ward	Martin		Pushing Technique Boundaries to Probe Conformational Polymorphism	518	THIRD FLOOR	137	29 August, Thur.	MS40
Ward	Suzanna		A toolkit for young crystallographers in need of more learning resources	531	FIRST FLOOR	73	27 August, Tue.	MS37 - How to address questions, doubts and struggles of a young crystallographer
Warren	Anna		The micro/nanofocus crystallography beamline VMXm at Diamond Light Source	650	GROUND FLOOR	9	28 August, Wed.	MS03
Weber	Thomas	Joohee Bang	Understanding complex order in thin film structures with the 3D-PDF method	527	FIRST FLOOR	44	27 August, Tue.	MS34 - Applications of 3D-PDF
Wehlander	Gabrielle		Exploring serial crystallography for capturing Michaelis complexes of a glucuronyl esterase involved in lignocellulose degradation	400	GROUND FLOOR	2	28 August, Wed.	MS03

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Weigel	Tina		Optimizing in Situ and Operando Experiments: Customized Sample Chamber with Heavy Load Goniometer	250	FIRST FLOOR	60	29 August, Thur.	MS25
Wicher	Barbara		Cocrystalline and co-amorphous systems of metformin with nonsteroidal anti-inflammatory drug meloxicam – synthesis, crystal structure and thermal properties	685	THIRD FLOOR	147	28 August, Wed.	MS32
Wiggers	Christin		Diffuse scattering in Sanidines	633	FIRST FLOOR	80	28 August, Wed.	MS17
Wiseman	Amy		Metagenomic mining for cold adapted phage enzymes	78	FIRST FLOOR	34	27 August, Tue.	MS6 - Structural studies in Enzymology
Woinska	Magdalena		Hirshfeld atom refinement for polymeric structures: MOFs and COFs	182	FIRST FLOOR	50	28 August, Wed.	MS11
Wolny	Janusz		Quarter century of the statistical method in crystallography	559	FIRST FLOOR	41	29 August, Thur.	MS14
Wong	Walter		Electron beam induced degradation of MAPbI ₃ revealed by low dose 3DED	316	THIRD FLOOR	110	27 August, Tue.	MS28 - Structural characterization of Energy Harvesting and Conversion Materials
Wu	Shitao		The Development and Application of 3D ED method in Crystalline Porous Materials	319	THIRD FLOOR	132	28 August, Wed.	MS30
Xu	Yizhi	Shaodi Li; Jiaoyan Xu; James Darby; Andrew J. Morris; Tomislav Friščić; Mihails Arhangelskis	Mechanochemical synthesis and structural characterization of hexafluorosilicate containing MOFs	701	THIRD FLOOR	156	29 August, Thur.	MS29
Yano	Naomine		Development of time-resolved structural analysis environment at SPring-8 BL41XU	165	GROUND FLOOR	10	27 August, Tue.	MS3 - Serial crystallography and dynamics/room temperature
Yoon	Hye-Jin		The effect of R518W mutation on the function of NPC1 cholesterol transport: Molecular dynamics simulation study	23	FIRST FLOOR	32	27 August, Tue.	MS6 - Structural studies in Enzymology
Yusenko	Kirill		Crystal Chemistry of Octahedral Rhodium(III) Chloroamines	248	FIRST FLOOR	94	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Zaytseva	Irina		Reactivity of the new caesium suboxometallate Cs ₇ MO ₄ (M = In, Sc)	329	FIRST FLOOR	78	27 August, Tue.	MS17 - Minerals and inorganic materials: state of art and new perspectives
Zhao	Yongsheng		PRESSURE INDUCED SUPERCONDUCTOR IN Rb ₂ Mo ₆ Se ₆	19	THIRD FLOOR	155	28 August, Wed.	MS12
Zheng	Shao-Liang		Addressing Crystallography Misconceptions for Chemistry Students	4	THIRD FLOOR	134	27 August, Tue.	MS41 - Approaches and tools for learning crystallography efficiently and avoiding misconceptions
Zolotarev	Pavel		A tool for the analysis of the bond strength anisotropy and search for the low-periodic substructures in crystalline solids	133	FIRST FLOOR	46	29 August, Thur.	MS22