

## Detailed MS Schedule (Tentative, as on 02 August 2017)

Date	Time	Hall	Theme	Microsymposium (MS)	ABS-Num.	Abstract Title	Presentation Type	Sequence	Chair/Author Name	Database ID
22-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-001: Analysis and validation of protein ligand structures			CHAIR	0	Bohdan Schneider	103
22-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-001: Analysis and validation of protein ligand structures			CHAIR	0	Andreas Heine	90
22-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-001: Analysis and validation of protein ligand structures	960	Small-molecule ligand/drug representation and validation in the Protein Data Bank	Oral 30 mins	1	Prof Genji Kurisu	658
22-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-001: Analysis and validation of protein ligand structures	185	Mogul: A tool to analyze protein bound ligand structures	Oral 30 mins	2	Dr Sivakumar Sekharan	283
22-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-001: Analysis and validation of protein ligand structures	752	The impact of crystallisation conditions on Structure-based drug design	Oral 30 mins	3	Dr Orly Dym	411
22-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-001: Analysis and validation of protein ligand structures	1058	Polder maps: Improving OMIT maps for ligand building and validation	Oral 30 mins	4	Dr Dorothee Claudia Liebschner	1312
22-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-001: Analysis and validation of protein ligand structures	488	Correcting the Record - Cofactor binding of Human Pyrroline-5-Carboxylate Reductase	Oral 15 mins	5	Prof Kurt L Krause	898
22-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-001: Analysis and validation of protein ligand structures	1162	Structure-based drug designing against Plasmepsins from Plasmodium falciparum	Oral 15 mins	6	Ms Vandana Mishra	1457

Date	Time	Hall	Theme	Microsymposium (MS)	ABS-Num.	Abstract Title	Presentation Type	Sequence	Chair/Author Name	Database ID
22-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-002: Crystallographic approach for designing new metal organic frameworks			CHAIR	0	Qiaowei Li	665
22-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-002: Crystallographic approach for designing new metal organic frameworks			CHAIR	0	Felipe Gandara	756
22-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-002: Crystallographic approach for designing new metal organic frameworks	186	Multicomponent Metal-Organic Frameworks	Oral 30 mins	1	Prof Shane Telfer	513
22-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-002: Crystallographic approach for designing new metal organic frameworks	1718	New Materials from the Packing and Linking of Supramolecular Nanoballs	Oral 30 mins	2	Prof Stuart Robert Batten	1855
22-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-002: Crystallographic approach for designing new metal organic frameworks	193	Harnessing the knowledge of metal-organic frameworks	Oral 30 mins	3	Dr Peter Andrew Wood	174
22-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-002: Crystallographic approach for designing new metal organic frameworks	576	SOME TITANIUM PHOSPHATES AS HOST MATERIALS: A CRYSTALLOGRAPHIC PERSPECTIVE	Oral 30 mins	4	Prof Santiago Garcia-Granda	186
22-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-002: Crystallographic approach for designing new metal organic frameworks	1806	Strategies for the Design of Functional MOFs: Addressing Energy-intensive Separations	Oral 30 mins	5	Prof Mohamed Eddaoudi	1422

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22-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-003: Crystal engineering solutions to improve pharmaceutical tableting			CHAIR	0	Thomas Hartman	2164
22-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-003: Crystal engineering solutions to improve pharmaceutical tableting			CHAIR	0	Changun Calvin Sun	1721
22-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-003: Crystal engineering solutions to improve pharmaceutical tableting	1689	Effect of crystallographic features on tableting behaviour of pharmaceutical actives	Oral 30 mins	1	Prof Arvind Bansal	1840
22-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-003: Crystal engineering solutions to improve pharmaceutical tableting	1882	Correspondence between crystal structures and tabletability in nitrofurantoin cocrystals	Oral 30 mins	2	Dr Venu R. Vangala	1485
22-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-003: Crystal engineering solutions to improve pharmaceutical tableting	1010	Aggregate elasticity and compaction performance: powder Brillouin light scattering	Oral 30 mins	3	Prof Lewis L. Stevens	1349
22-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-003: Crystal engineering solutions to improve pharmaceutical tableting	481	Synergistic enhancement of tabletability and physicochemical properties through cocrystallization	Oral 30 mins	4	Dr Srinivasulu Aitipamula	879
22-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-003: Crystal engineering solutions to improve pharmaceutical tableting	556	Synthonic-Molecular Modelling of Pentaerythritol and Pentaerythritol Tetranitrate Slip Systems	Oral 15 mins	5	Dr Siti Fatimah Ibrahim	970
22-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-003: Crystal engineering solutions to improve pharmaceutical tableting	1277	Impact of microstructure on compaction behaviour of aspirin-paracetamol eutectic system	Oral 15 mins	6	Mr Sandeep S. Zode	1431
22-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-004: Novel direct methods for electron diffraction and imaging			CHAIR	0	Stavros Nicolopoulos	1181
22-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-004: Novel direct methods for electron diffraction and imaging			CHAIR	0	Partha Ghoshal	258
22-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-004: Novel direct methods for electron diffraction and imaging	1968	From Low Dose In-Line Electron Holography to Atomic Resolution Tomography	Oral 30 mins	1	Prof Fu-Rong Chen	2396

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22-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-004: Novel direct methods for electron diffraction and imaging	1417	Investigation of layered and porous nanomaterials by electron diffraction tomography	Oral 30 mins	2	Mr Yasar Krysiak	1646
22-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-004: Novel direct methods for electron diffraction and imaging	1137	Determination of very beam-sensitive zeolite ITQ-57 by energy-filtered Timepix data	Oral 30 mins	3	Dr Enrico Mugnaioli	1449
22-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-004: Novel direct methods for electron diffraction and imaging	495	Accurate Determination of Crystal Orientation from Rotation Electron Diffraction Data	Oral 15 mins	4	Mr Bin Wang	731
22-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-004: Novel direct methods for electron diffraction and imaging	511	Electron Crystallography of Protein Nano-Crystals	Oral 15 mins	5	Dr Igor Nederlof	922
22-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-004: Novel direct methods for electron diffraction and imaging	1450	Solving an unknown phase in a HP/HT Sr-Cu-Ge-O sample	Oral 15 mins	6	Dr Holger Klein	1662
22-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-005: Total scattering			CHAIR	0	Eduardo Granado	1671
22-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-005: Total scattering			CHAIR	0	Katherine Page	2009
22-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-005: Total scattering	1603	Anomalously large magnetoresistance in an antiferromagnet	Oral 30 mins	1	Prof Despina Louca	1754
22-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-005: Total scattering	1240	The Automated XPDF Beamline at Diamond Light Source	Oral 30 mins	2	Dr Philip Anthony Chater	1533
22-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-005: Total scattering	90	Local Structure of Bi4TaO8Cl Nanophotocatalyst by NPDF Analysis	Oral 30 mins	3	Dr Nalini Ganapathy Sundaram	58
22-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-005: Total scattering	30	Local structure of dielectric framework materials	Oral 30 mins	4	Dr Anthony Phillips	85
22-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-005: Total scattering	384	Local structure study during hydrogenation by time-resolved x-ray total scattering	Oral 30 mins	5	Dr Akihiko Machida	795

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22-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-006: Computational materials design			CHAIR	0	Samrath Lal Chaplot	2065
22-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-006: Computational materials design			CHAIR	0	Artem Oganov	550
22-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-006: Computational materials design	57	Multilevel topological analysis in application to design of coordination networks	Oral 30 mins	1	Dr Eugeny V. Alexandrov	196
22-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-006: Computational materials design	1268	Theoretical and experimental screening methods for functional materials design	Oral 30 mins	2	Dr Matthew Dunstan	1544
22-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-006: Computational materials design	1931	Microscopic mechanisms of the pressure-induced amorphization of SiO <sub>2</sub>	Oral 30 mins	3	Prof Sandro Scandolo	1583
22-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-006: Computational materials design	1090	Ab initio lattice dynamics for materials design and characterisation	Oral 30 mins	4	Dr Jonathan Michael Skelton	1416
22-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-006: Computational materials design	811	Uranium phase diagram built using machine learning interatomic potential	Oral 15 mins	5	Mr Ivan Kruglov	1199
22-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-006: Computational materials design	2055	A Cognitive Computing Environment for Materials Research	Oral 15 mins	6	Dr John Rodgers	2278
22-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-007: Topology and symmetry of modular structures			CHAIR	0	Isabella Pignatelli	689
22-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-007: Topology and symmetry of modular structures			CHAIR	0	Sergey V. Krivovichev	1527
22-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-007: Topology and symmetry of modular structures	276	Symmetry classification of modular structures with groupoid families	Oral 30 mins	1	Dr Berthold Stöger	668
22-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-007: Topology and symmetry of modular structures	1107	From anion-centered tetrahedra to modular chemistry of Bi/La oxysalts.	Oral 30 mins	2	Dr Marie Colmont	1433
22-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-007: Topology and symmetry of modular structures	1065	'Hydrocerussite' puzzle	Oral 30 mins	3	Dr Oleg Siidra	1395
22-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-007: Topology and symmetry of modular structures	87	Multidimensional structural variation in the cyanotrichite family of merotypes	Oral 15 mins	4	Dr Stuart James Mills	79

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22-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-007: Topology and symmetry of modular structures	608	Modular crystallography of novel copper selenites and selenates: experimental mineralogy	Oral 15 mins	5	Dr Vadim M. Kovrugin	420
22-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-007: Topology and symmetry of modular structures	1219	Layered tellurite-chlorides obtained by CVT: simple way for complex structures	Oral 15 mins	6	Ms Diana Olegovna Nekrasova	409
22-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-007: Topology and symmetry of modular structures	1403	Structural variations of uranium compounds with nitrate anions	Oral 15 mins	7	Ms Anastasiya Igorevna Zadoya	428
22-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-008: Magnetic order and its consequences			CHAIR	0	Arsene Goukassov	910
22-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-008: Magnetic order and its consequences			CHAIR	0	Takashi Kamiyama	1989
22-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-008: Magnetic order and its consequences	503	Bilayered crystal of magnetic monopoles and multiferroicity in spin ice	Oral 30 mins	1	Dr Arsene Goukassov	910
22-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-008: Magnetic order and its consequences	1875	Some Topics in Structural Change on Magnetic Order	Oral 30 mins	2	Prof Takashi Kamiyama	1989
22-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-008: Magnetic order and its consequences	1286	Premartensitic and Martensitic Phase Transitions in Magnetic Shape Memory Alloys	Oral 30 mins	3	Dr Sanjay Singh	1504
22-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-008: Magnetic order and its consequences	1458	Understanding multiferroicity in the new (ND <sub>4</sub> ) <sub>2</sub> FeCl <sub>5</sub> (D <sub>2</sub> O) molecular magnet	Oral 30 mins	4	Prof Javier Campo	1667
22-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-008: Magnetic order and its consequences	512	Unconventional magnetic order in GeFe <sub>2</sub> O <sub>4</sub>	Oral 15 mins	5	Ms Giuditta Perversi	924
22-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-008: Magnetic order and its consequences	539	Magnetic phase diagram of Mn(Ru-Rh)As - magnetoelastic and electronic properties	Oral 15 mins	6	Mr Ryszard Zach	952

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22-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-009: Enzymes, mechanism and drug design			CHAIR	0	Marjolein Thunnissen	1607
22-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-009: Enzymes, mechanism and drug design			CHAIR	0	Anthony Addlagatta	744
22-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-009: Enzymes, mechanism and drug design	381	How oxygenases catalyze a variety of reactions?	Oral 30 mins	1	Prof S Ramaswamy	791
22-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-009: Enzymes, mechanism and drug design	662	Time-resolved XFEL crystallography and spectroscopy of cytochrome c oxidase	Oral 30 mins	2	Dr Minoru Kubo	1078
22-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-009: Enzymes, mechanism and drug design	1408	Validation of a 96-Fragment Library for Crystallographic Screening	Oral 30 mins	3	Prof Andreas Heine	90
22-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-009: Enzymes, mechanism and drug design	1791	Proton transfer inhibition by molecular anion substitutions in Photosystem II	Oral 15 mins	4	Dr Yasufumi Umena	1901
22-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-009: Enzymes, mechanism and drug design	92	Structure guided design of aromatic biosensors for water quality monitoring	Oral 15 mins	5	Ms Shamayeeta Ray	302
22-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-009: Enzymes, mechanism and drug design	1873	Functional and structural exploration of the Abyssomicin C synthetic pathway	Oral 15 mins	6	Dr Alice Parnell	1987
22-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-009: Enzymes, mechanism and drug design	1426	Design of peptidic inhibitors targeting the dimerization interface of galectins	Oral 15 mins	7	Dr Jacinthe Gagnon	471
22-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-010: Membrane proteins, lipid-protein interactions and membrane fusion			CHAIR	0	Arun Shukla	2033
22-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-010: Membrane proteins, lipid-protein interactions and membrane fusion			CHAIR	0	Margarida Archer	1297
22-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-010: Membrane proteins, lipid-protein interactions and membrane fusion	489	Structural Dynamics of Membrane Proteins	Oral 30 mins	1	Prof So Iwata	826

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22-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-010: Membrane proteins, lipid-protein interactions and membrane fusion	1348	Interfacial lipids as modulator of membrane protein oligomerisation	Oral 30 mins	2	Dr Kallol Gupta	925
22-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-010: Membrane proteins, lipid-protein interactions and membrane fusion	834	Challenges and Opportunities in Structure Determination of Membrane Proteins	Oral 30 mins	3	Dr Isabel Moraes	1218
22-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-010: Membrane proteins, lipid-protein interactions and membrane fusion	477	Insights into Neurotransmitter Release from the Structure of Munc13-1 C1C2BMUN	Oral 30 mins	4	Prof Diana R Tomchick	873
22-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-010: Membrane proteins, lipid-protein interactions and membrane fusion	646	Structures of Bak with Lipids: Implications for Pore Formation	Oral 15 mins	5	Dr Peter Czabotar	1067
22-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-010: Membrane proteins, lipid-protein interactions and membrane fusion	1598	Charaterising PC/Cholesterol Supported Lipid Bilayers and Interactions with Human HDL	Oral 15 mins	6	Ms Sarah Hannah Anne Waldie	1748
22-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-011: Applications of post-synthesis modified metal-organic frameworks			CHAIR	0	Myoung Soo Lah	2030
22-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-011: Applications of post-synthesis modified metal-organic frameworks			CHAIR	0	Praveen Thallapally	358
22-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-011: Applications of post-synthesis modified metal-organic frameworks	1866	UUltra-Microporous MOFs for Selective CO2 Capture from Industrial Gas Mixtures	Oral 30 mins	1	Dr Vaidhyanathan Ramanathan	1982
22-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-011: Applications of post-synthesis modified metal-organic frameworks	993	SC-SC Transformation of 2D MOFs to 3D by [2+2] Photodimerization	Oral 30 mins	2	Prof Hoi Ri Moon	1332
22-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-011: Applications of post-synthesis modified metal-organic frameworks	1973	Modelling of MOFs for energy and environment-related applications	Oral 30 mins	3	Prof Guillaume Maurin	2131
22-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-011: Applications of post-synthesis modified metal-organic frameworks	1580	Supramolecular Construction of an Aldehyde-Functionalized Cyclobutane in the Solid State	Oral 30 mins	4	Ms Shalisa Malane Oburn	1733



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22-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-011: Applications of post-synthesis modified metal-organic frameworks	422	Photochromic Metal Organic Frameworks for Inkless and Erasable Printing	Oral 30 mins	5	Mr Bikash Garai	743
22-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-012: Structure-property correlation in pharmaceutical solids			CHAIR	0	Javier Ellena	766
22-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-012: Structure-property correlation in pharmaceutical solids			CHAIR	0	Christian W. Lehmann	2051
22-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-012: Structure-property correlation in pharmaceutical solids	898	Solvent-free methods for controllable synthesis of metastable pharmaceutical solids	Oral 30 mins	1	Dr Krunoslav Uzarevic	1150
22-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-012: Structure-property correlation in pharmaceutical solids	717	Correlating crystal structure, Nanomechanical, and Compaction behavior of Febuxostat polymorphs	Oral 30 mins	2	Mr Jayprakash Amarpal Yadav	1124
22-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-012: Structure-property correlation in pharmaceutical solids	640	Pharmaceutical solid solutions of antiretroviral drugs	Oral 30 mins	3	Prof Alejandro Pedro Ayala	80
22-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-012: Structure-property correlation in pharmaceutical solids	990	Impact of differential surface anisotropy on Biopharmaceutical Performance of Celecoxib	Oral 30 mins	4	Ms Poonam Singh Thakur	1023
22-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-012: Structure-property correlation in pharmaceutical solids	1578	Structural origin of superior plasticity and tableability of theophylline monohydrate	Oral 15 mins	5	Prof Changquan Calvin Sun	1721
22-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-012: Structure-property correlation in pharmaceutical solids	210	Can predicted solid form landscapes provide insight into structure-property correlations?	Oral 15 mins	6	Dr Andrew Gerrard Patrick Maloney	172
22-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-013: Quantitative electron imaging and tomography			CHAIR	0	Andreas Rosenauer	311
22-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-013: Quantitative electron imaging and tomography			CHAIR	0	Eric Van Cappellen	417
22-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-013: Quantitative electron imaging and tomography	52	Integrated Differential Phase Contrast (iDPC) STEM	Oral 30 mins	1	Dr Ivan Ladic	187

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22-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-013: Quantitative electron imaging and tomography	213	Mapping atomic electric fields and charge densities by four-dimensional STEM	Oral 30 mins	2	Dr Knut Müller-Caspary	438
22-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-013: Quantitative electron imaging and tomography	342	Electron tomography – 3D atomic, elemental and field mapping	Oral 30 mins	3	Dr Georg Haberfehlner	749
22-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-013: Quantitative electron imaging and tomography	1236	Imaging charge transfer in crystals using electron ptychography	Oral 30 mins	4	Prof Peter Nellist	1269
22-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-013: Quantitative electron imaging and tomography	602	Nanoscale Strain Tomography by Scanning Precession Electron Diffraction	Oral 30 mins	5	Mr Duncan N. Johnstone	1027
22-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-014: Advanced neutron sources in biological and materials sciences			CHAIR	0	Despina Louca	1754
22-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-014: Advanced neutron sources in biological and materials sciences	2021	News and Perspectives of the European Spallation Source	Oral 30 mins	1	Prof Ken Holst Andersen	316
22-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-014: Advanced neutron sources in biological and materials sciences	595	Current Status of J-PARC MLF	Oral 30 mins	2	Prof Toshiji Kanaya	1015
22-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-014: Advanced neutron sources in biological and materials sciences	1732	The neutron powder diffractometer DREAM at the ESS	Oral 30 mins	3	Dr Werner Schweika	1830
22-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-014: Advanced neutron sources in biological and materials sciences	1476	D19: a neutron diffractometer for small proteins and chemical crystallography	Oral 30 mins	4	Dr Estelle Mossou	1677
22-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-014: Advanced neutron sources in biological and materials sciences	1941	New Science Capabilities at Current and Proposed U.S. Neutron Sources	Oral 30 mins	5	Dr Katharine Lynn Page	2009

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22-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-015: In-situ and in-operando characterization of energy materials			CHAIR	0	Diego Lamas	1323
22-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-015: In-situ and in-operando characterization of energy materials			CHAIR	0	Yang Ren	2083
22-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-015: In-situ and in-operando characterization of energy materials	278	Composition-Structure-Activity Relationship for Fuel Cell Catalysts by in operando XRD	Oral 30 mins	1	Prof Valeri Petkov	671
22-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-015: In-situ and in-operando characterization of energy materials	236	In-situ characterization of energy materials by neutron diffraction	Oral 30 mins	2	Prof Jose Antonio Alonso	591
22-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-015: In-situ and in-operando characterization of energy materials	1169	Probing structural distortions with new high-precision resonant X-ray diffraction approach	Oral 15 mins	3	Dr Matthias Zschornak	1479
22-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-015: In-situ and in-operando characterization of energy materials	1452	Electrochemical cells for neutron diffraction study of Li/Na-ion electrode materials	Oral 15 mins	4	Dr Ivan Bobrikov	1418
22-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-015: In-situ and in-operando characterization of energy materials	613	Structure Property correlation in SOFC & SOEC materials	Oral 15 mins	5	Prof David Gordon Billing	1031
22-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-015: In-situ and in-operando characterization of energy materials	763	In operando data of Li-Ion batteries from XRPD laboratory diffractometers	Oral 15 mins	6	Dr Thomas Degen	127
22-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-015: In-situ and in-operando characterization of energy materials	1954	Unravelling the photoredox pathways in CO2 photoreduction by artificial photosynthesis	Oral 15 mins	7	Dr Víctor Antonio De La Peña O'Shea	1669
22-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-015: In-situ and in-operando characterization of energy materials	1548	A Laue Diffractometer for ambient and non-ambient Neutron Structural Analysis	Oral 15 mins	8	Dr Michael Tovar	1718

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22-08-2017	1455-1730	MR 2.01	Special Activities	MS-016: New approaches in crystallographic teaching			CHAIR	0	Louise Dawe	1043
22-08-2017	1455-1730	MR 2.01	Special Activities	MS-016: New approaches in crystallographic teaching			CHAIR	0	Peter Moeck	78
22-08-2017	1455-1730	MR 2.01	Special Activities	MS-016: New approaches in crystallographic teaching	632	Interactive teaching of crystallography using Jmol	Oral 30 mins	1	Prof Robert Mark Hanson	678
22-08-2017	1455-1730	MR 2.01	Special Activities	MS-016: New approaches in crystallographic teaching	772	Crystallography online by the Bilbao Crystallographic Server	Oral 30 mins	2	Dr Gemma De La Flor Martin	521
22-08-2017	1455-1730	MR 2.01	Special Activities	MS-016: New approaches in crystallographic teaching	918	Crystallography Open Database for teaching	Oral 30 mins	3	Dr Saulius Grazulis	1287
22-08-2017	1455-1730	MR 2.01	Special Activities	MS-016: New approaches in crystallographic teaching	230	Making crystal structure an everyday thing – Crystallography365 and beyond	Oral 30 mins	4	Dr Helen Elizabeth Maynard-Casely	514
22-08-2017	1455-1730	MR 2.01	Special Activities	MS-016: New approaches in crystallographic teaching	189	A 3D Approach to Teaching Chemistry	Oral 15 mins	5	Dr Amy A. Sarjeant	171
22-08-2017	1455-1730	MR 2.01	Special Activities	MS-016: New approaches in crystallographic teaching	460	Teaching Structural Biology, Bioinformatics and Evolution to High School Students	Oral 15 mins	6	Dr Bill Duax	858
22-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-017: Extending the boundaries of crystallography			CHAIR	0	Manuel Loquias	372
22-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-017: Extending the boundaries of crystallography			CHAIR	0	Mois I Aroyo	929
22-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-017: Extending the boundaries of crystallography	217	Quasicrystals. What do we know - what can we know?	Oral 30 mins	1	Prof Walter Steurer	94
22-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-017: Extending the boundaries of crystallography	654	3D euclidean crystallography and hyperbolic orbifolds	Oral 30 mins	2	Dr Stephen Timothy Hyde	724
22-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-017: Extending the boundaries of crystallography	1341	Two extensions: Bronze-mean quasicrystal and crystals on saddle-shaped surfaces	Oral 30 mins	3	Prof Tomonari Dotera	1598
22-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-017: Extending the boundaries of crystallography	1774	Understanding local structure in amorphous precursors using electron nano diffraction	Oral 30 mins	4	Dr Espen Drath Boejesen	1903

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22-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-017: Extending the boundaries of crystallography	204	Extreme cooperative swelling in topologically disordered fibre entanglements	Oral 15 mins	5	Mr Alistair Overy	548
22-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-017: Extending the boundaries of crystallography	868	Mapping the trajectory of proton transfer via experimental electron density.	Oral 15 mins	6	Ms Lorraine Andrade Malaspina	571
22-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-018: Ion transport			CHAIR	0	Nakagawa Atsushi	956
22-08-2017	1455-1730	MR 2.03-2.04	Macromolecules (Function)	MS-018: Ion transport			CHAIR	0	Daniel Minor	2149
22-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-018: Ion transport	1982	Panning for precious metals: Mechanics of a transition metal transporter	Oral 30 mins	1	Prof Rachele Gaudet	2154
22-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-018: Ion transport	2018	Deciphering ligand induced conformational changes in the Sodium Galactose Transporter	Oral 30 mins	2	Prof Jeff Abramson	2212
22-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-018: Ion transport	2034	Molecular mechanism of the Mg <sup>2+</sup> channel MgT <sub>E</sub>	Oral 30 mins	3	Prof Osamu Nureki	1811
22-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-018: Ion transport	2101	Driving a wedge into the TREK channel heart	Oral 30 mins	4	Prof Daniel Minor	2149
22-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-018: Ion transport	2102	Structural Insight of Zinc Binding of Hv1/VSOP in Resting State	Oral 30 mins	5	Prof Nakagawa Atsushi	956
23-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-019: Interactions between proteins and nucleic acids			CHAIR	0	Markus Wahl	1860
23-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-019: Interactions between proteins and nucleic acids			CHAIR	0	Barnali Chaudhuri	349
23-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-019: Interactions between proteins and nucleic acids	132	Determination of reaction intermediates and catalytic mechanism by X-ray Diffraction	Oral 30 mins	1	Dr Wei Yang	429
23-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-019: Interactions between proteins and nucleic acids	1770	HU multimerization shift controls nucleoid compaction	Oral 30 mins	2	Dr Michal Hammel	1899
23-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-019: Interactions between proteins and nucleic acids	1937	Molecular mechanism of CRISPR	Oral 30 mins	3	Prof Osamu Nureki	1811

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23-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-019: Interactions between proteins and nucleic acids	1365	Parsimonious DNA target-site recognition by Grh/CP2 transcription factors	Oral 30 mins	4	Prof Udo Heinemann	1616
23-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-019: Interactions between proteins and nucleic acids	1836	Structural Insights into Plasticity of DNA-Protein Interactions in Tetracycline Receptors	Oral 15 mins	5	Prof Ruchi Anand	1964
23-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-019: Interactions between proteins and nucleic acids	1790	Crystal structure of tetrameric Arabidopsis MYC2-DNA complex	Oral 15 mins	6	Prof Xiao-Dong Su	1017
23-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-020: Controlling dimensions of porous crystalline polymers			CHAIR	0	Wei Wang	1338
23-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-020: Controlling dimensions of porous crystalline polymers			CHAIR	0	P S Mukherjee	1177
23-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-020: Controlling dimensions of porous crystalline polymers	207	Heteropore COFs: An Emerging Class of Crystalline Hierachically Porous Polymers	Oral 30 mins	1	Prof Xin Zhao	553
23-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-020: Controlling dimensions of porous crystalline polymers	1671	Stimuli-responsive Functional Metal-Organic Frameworks	Oral 30 mins	2	Prof Tapas Kumar Maji	1818
23-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-020: Controlling dimensions of porous crystalline polymers	996	A Dynamic Three-Dimensional Covalent Organic Framework	Oral 30 mins	3	Prof Wei Wang	1338
23-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-020: Controlling dimensions of porous crystalline polymers	159	Structural dynamism in metal-organic framework leading to their better functionality	Oral 15 mins	4	Dr Debajyoti Ghoshal	107
23-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-020: Controlling dimensions of porous crystalline polymers	1614	STRUCTURAL REGULATION OF LUMINESCENT AND MAGNETIC PROPERTIES OF MOFS	Oral 15 mins	5	Prof Tatiana Timofeeva	1763
23-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-020: Controlling dimensions of porous crystalline polymers	1840	Neutral Polyhedral Pd(II) Cages Supported by Tris(imido)phosphate Trianions	Oral 15 mins	6	Dr Boomishankar Ramamoorthy	1967
23-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-020: Controlling dimensions of porous crystalline polymers	754	Pd(II)-LMOF FOR THE SENSING OF MOLECULAR HYDROGEN IN GAS PHASE	Oral 15 mins	7	Dr Katherine Chulvi-Iborra	785
23-08-2017	1030-1305	Hall 6	Special Activities	MS-021: Terminology issues in crystal engineering			CHAIR	0	Christer Aakeröy	516

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23-08-2017	1030-1305	Hall 6	Special Activities	MS-021: Terminology issues in crystal engineering			CHAIR	0	Carolyn P. Brock	602
23-08-2017	1030-1305	Hall 6	Special Activities	MS-021: Terminology issues in crystal engineering	37	IUPAC definition of the hydrogen bond. Terminology and nomenclature	Oral 30 mins	1	Prof Gautam R. Desiraju	110
23-08-2017	1030-1305	Hall 6	Special Activities	MS-021: Terminology issues in crystal engineering	629	IUPAC definition of the halogen bond	Oral 30 mins	2	Prof Pierangelo Metrangolo	1044
23-08-2017	1030-1305	Hall 6	Special Activities	MS-021: Terminology issues in crystal engineering	650	MOFs - What is in the name?	Oral 30 mins	3	Prof Jagadese J Vittal	1070
23-08-2017	1030-1305	Hall 6	Special Activities	MS-021: Terminology issues in crystal engineering	1566	Polymorphs, pseudopolymorphs, and the crystal engineer: friends and foes	Oral 30 mins	4	Prof Leonard Richard MacGillivray	1690
23-08-2017	1030-1305	Hall 6	Special Activities	MS-021: Terminology issues in crystal engineering	1699	Co-crystal: A simple term with many interpretations	Oral 30 mins	5	Prof Christer Bjorn Aakeroy	516
23-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-023: Synchrotron and XFEL for materials at ambient and extreme conditions			CHAIR	0	John Tse	1557
23-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-023: Synchrotron and XFEL for materials at ambient and extreme conditions			CHAIR	0	Yasuo Ohishi	2073
23-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-023: Synchrotron and XFEL for materials at ambient and extreme conditions	1990	Ultrafast XRD observation of laser-shock induced lattice dynamics	Oral 30 mins	1	Dr Norimasa Ozaki	2169
23-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-023: Synchrotron and XFEL for materials at ambient and extreme conditions	1925	Sample Extractor for Serial Crystallography at XFELs and Synchrotron sources	Oral 30 mins	2	Dr Irimpan Mathews	2035
23-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-023: Synchrotron and XFEL for materials at ambient and extreme conditions	1409	In-situ synchrotron diffraction study of precipitations in liquid jet	Oral 30 mins	3	Mr Ahmed S. A. Mohammed	1629
23-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-023: Synchrotron and XFEL for materials at ambient and extreme conditions	827	Pioneering remote-access use of Diamond beamline I19	Oral 30 mins	4	Prof William Clegg	475

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23-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-023: Synchrotron and XFEL for materials at ambient and extreme conditions	1733	MCX@Elettra: Powder diffraction in ambient and non ambient conditions	Oral 30 mins	5	Dr Jasper Rikkert Plaisier	1874
23-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-024: NMR Crystallography and related methods			CHAIR	0	Manish Mehta	2308
23-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-024: NMR Crystallography and related methods	1908	Predicting and refining crystal structures with NMR data	Oral 30 mins	1	Dr James Harper	2013
23-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-024: NMR Crystallography and related methods	1503	Solid-State NMR Crystallography: from Catalytic Active Complexes to Enzymes	Oral 30 mins	2	Prof Gerd Buntkowsky	1687
23-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-024: NMR Crystallography and related methods	1967	NMR Crystallography: A Perspective	Oral 30 mins	3	Prof Perunthiruthy Madhu	2119
23-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-024: NMR Crystallography and related methods	845	New Developments in Surface-Enhanced Solid-State NMR Spectroscopy and their Applications	Oral 30 mins	4	Dr Sachin Rama Chaudhari	1090
23-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-024: NMR Crystallography and related methods	2042	Determination of crystalline forms by solid-state NMR and electron diffraction	Oral 15 mins	5	Dr Yusuke Nishiyama	2041
23-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-024: NMR Crystallography and related methods	2096	Structure, Disorder and Function of Supramolecular Polymer Additives	Oral 15 mins	6	Prof Juergen Senker	2487
23-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-025: Crystallography of battery materials			CHAIR	0	Prabeer Barpanda	64
23-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-025: Crystallography of battery materials	354	Probing Electrode Materials Bulk and Interfacial Processes with NMR Spectroscopy	Oral 30 mins	1	Dr Michal Leskes	764
23-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-025: Crystallography of battery materials	1073	Enhanced energy density in oxides and alluaudites battery materials	Oral 30 mins	2	Dr Prabeer Barpanda	64
23-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-025: Crystallography of battery materials	528	Local structure of Li4-xMn2O5 high capacity cathode probed by PDF	Oral 30 mins	3	Dr Maria Diaz-Lopez	939
23-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-025: Crystallography of battery materials	364	Current status of iMATERIA and recent result of LIB research	Oral 30 mins	4	Prof Toru Ishigaki	774
23-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-025: Crystallography of battery materials	388	Assessment of potential Al ion conductors from large crystallographic databases	Oral 15 mins	5	Mr Falk Meutzner	730



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23-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-025: Crystallography of battery materials	871	Crystal Structures and Electrochemical Properties of the Battery Materials NaxM3(PO4)3	Oral 15 mins	6	Dr Hamdi Ben Yahia	1249
23-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-026: A bridge between two worlds: Graphs as structural descriptors			CHAIR	0	Hamilton Barbosa Napolitano	949
23-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-026: A bridge between two worlds: Graphs as structural descriptors			CHAIR	0	Bernd Souvignier	2161
23-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-026: A bridge between two worlds: Graphs as structural descriptors	240	Labelled quotient graphs and topological features in crystal structures	Oral 30 mins	1	Prof Jean Guillaume Eon	599
23-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-026: A bridge between two worlds: Graphs as structural descriptors	573	Vertex-transitive monocoronal tilings from isohedral tilings	Oral 30 mins	2	Mr Eduard Camangian Taganap	994
23-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-026: A bridge between two worlds: Graphs as structural descriptors	1208	Short-range order analyses of the amorphous-crystalline silicates using graph theory	Oral 30 mins	3	Dr Olga Sidorova	1520

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23-08-2017	1030-1305	MR 2.03-2.04	Instrumentation techniques and/or Computation	MS-027: Synchrotron-based X-ray techniques and the environment			CHAIR	0	Richard Garrett	2417
23-08-2017	1030-1305	MR 2.03-2.04	Instrumentation techniques and/or Computation	MS-027: Synchrotron-based X-ray techniques and the environment			CHAIR	0	Hugh Harris	2103
23-08-2017	1030-1305	MR 2.03-2.04	Instrumentation techniques and/or Computation	MS-027: Synchrotron-based X-ray techniques and the environment	964	Towards a mechanistic understanding of mercury –microbe/mineral interactions	Oral 30 mins	1	Dr Bhoopesh Mishra	53
23-08-2017	1030-1305	MR 2.03-2.04	Instrumentation techniques and/or Computation	MS-027: Synchrotron-based X-ray techniques and the environment	1962	Cryo micro-spectroscopy at ID21 for environmental sciences	Oral 30 mins	2	Dr Marine Cotte	1142
23-08-2017	1030-1305	MR 2.03-2.04	Instrumentation techniques and/or Computation	MS-027: Synchrotron-based X-ray techniques and the environment	2086	X-ray absorption spectroscopy for lead speciation of dispersed mine waste	Oral 30 mins	3	Prof Barry Neil Noller	2416
23-08-2017	1030-1305	MR 2.03-2.04	Instrumentation techniques and/or Computation	MS-027: Synchrotron-based X-ray techniques and the environment	2001	Synchrotron high-energy x-rays for materials research with complex sample environments	Oral 30 mins	4	Dr Yang Ren	2083
23-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-028: Long wavelength applications in macromolecular crystallography			CHAIR	0	Christoph Mueller-Dieckmann	2038
23-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-028: Long wavelength applications in macromolecular crystallography			CHAIR	0	Dorothee Liebschner	1312
23-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-028: Long wavelength applications in macromolecular crystallography	893	Making routine native SAD a reality	Oral 30 mins	1	Dr Vincent Olieric	470
23-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-028: Long wavelength applications in macromolecular crystallography	1149	The long-wavelength macromolecular crystallography beamline I23 at Diamond Light Source	Oral 30 mins	2	Dr Armin Wagner	1472
23-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-028: Long wavelength applications in macromolecular crystallography	1899	Exploiting wavelength longer than 3 Å for native SAD phasing	Oral 30 mins	3	Dr Naohiro Matsugaki	1958
23-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-028: Long wavelength applications in macromolecular crystallography	1369	Maximum likelihood methods in DIALS	Oral 30 mins	4	Mr James Parkhurst	1450

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23-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-028: Long wavelength applications in macromolecular crystallography	741	Experimental phasing at low energy at EMBL beamline P13	Oral 30 mins	5	Dr Guillaume Pompidor	1148

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23-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-029: Porous framework materials for gas adsorption			CHAIR	0	Hoi Ri Moon	1332
23-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-029: Porous framework materials for gas adsorption			CHAIR	0	Sunil Varughese	324
23-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-029: Porous framework materials for gas adsorption	1330	Coordination Exchanges in Metal-Organic Frameworks	Oral 30 mins	1	Prof Nak Cheon Jeong	1590
23-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-029: Porous framework materials for gas adsorption	641	CO2 release from Metal-Organic Frameworks triggered by external stimuli	Oral 30 mins	2	Dr Haiqing Li	878
23-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-029: Porous framework materials for gas adsorption	1647	Reactive sites for Adsorption and catalysis in MOFs	Oral 30 mins	3	Prof Christian James Doonan	1799
23-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-029: Porous framework materials for gas adsorption	994	FUNCTIONALIZATION INDUCED BREATHING CONTROL IN FLEXIBLE MOFS	Oral 30 mins	4	Dr Tanay Kundu	1334
23-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-029: Porous framework materials for gas adsorption	1470	In situ CO2 adsorption by the (poly)azolate MOF Fe2BPEB3	Oral 15 mins	5	Dr Carlotta Giacobbe	1674
23-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-029: Porous framework materials for gas adsorption	337	Design of Porous MOFs for gas storage applications	Oral 15 mins	6	Mr Sandeep Singh Dhankhar	685
23-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-030: Crystallization mechanisms of small molecule organic materials			CHAIR	0	Jaime Gomez Morales	646
23-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-030: Crystallization mechanisms of small molecule organic materials			CHAIR	0	Raj Suryanarayana	1762
23-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-030: Crystallization mechanisms of small molecule organic materials	1970	Solution Speciation and Implication on Nucleation Mechanism	Oral 30 mins	1	Prof Tonglei Li	2129
23-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-030: Crystallization mechanisms of small molecule organic materials	726	The Crystal Morphology and Growth Kinetic Mechanisms of Para-AminoBenzoic Acid	Oral 30 mins	2	Dr Ian Rosbottom	1131
23-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-030: Crystallization mechanisms of small molecule organic materials	742	Unstable amorphous cerium oxalate precipitation in concentrated HNO3 media	Oral 30 mins	3	Dr Isaac Rodriguez-Ruiz	1151

Date	Time	Hall	Theme	Microsymposium (MS)	ABS-Num.	Abstract Title	Presentation Type	Sequence	Chair/Author Name	Database ID
23-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-030: Crystallization mechanisms of small molecule organic materials	379	Laser Assisted Crystallization: An alternative tool to crystallize biomolecules	Oral 30 mins	4	Dr Abdul Ajees Abdul Salam	784
23-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-030: Crystallization mechanisms of small molecule organic materials	1441	Enantiotropic phase transition in a molecular solid involving Z'=12	Oral 30 mins	5	Dr Ilia Guzei	1658
23-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-031: Nanoparticles / nanostructures			CHAIR	0	N. Ravishankar	2034
23-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-031: Nanoparticles / nanostructures	1946	The chemistry of nucleation	Oral 30 mins	1	Prof Bo Brummerstedt Iversen	1784
23-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-031: Nanoparticles / nanostructures	882	Nanostructured MOFs through defect engineering	Oral 30 mins	2	Dr Matthew Cliffe	523
23-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-031: Nanoparticles / nanostructures	1517	Real and reciprocal space electron tomography reveals structure and vacancies	Oral 30 mins	3	Dr Tom Willhammar	1661
23-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-031: Nanoparticles / nanostructures	338	Crystallographic investigation of metallic and bimetallic nanoparticles	Oral 15 mins	4	Dr Oleg Prymak	740
23-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-031: Nanoparticles / nanostructures	798	Nanoparticle and nanocluster structures at atomic resolution – even hydrides!	Oral 15 mins	5	Dr Alison Jeanine Edwards	1186
23-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-031: Nanoparticles / nanostructures	1905	Resolving the atomistic structure and morphology of functional nanomaterials	Oral 15 mins	6	Dr Katharine Lynn Page	2009
23-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-031: Nanoparticles / nanostructures	1986	Tuning of Metal Oxides Nanostructures under Soft Hydrothermal Conditions	Oral 15 mins	7	Prof Kullaiah Byrappa	2160
23-08-2017	1455-1730	MR 1.05	Special Activities	MS-032: Crystallography courses around the world			CHAIR	0	Annalisa Guerri	113
23-08-2017	1455-1730	MR 1.05	Special Activities	MS-032: Crystallography courses around the world			CHAIR	0	Juan Manuel Garcia Ruiz	2042
23-08-2017	1455-1730	MR 1.05	Special Activities	MS-032: Crystallography courses around the world	182	A World-Wide Education in Crystallography	Oral 15 mins	1	Dr Amy A. Sarjeant	171
23-08-2017	1455-1730	MR 1.05	Special Activities	MS-032: Crystallography courses around the world	828	Growing a new generation of crystallographers across Europe and beyond	Oral 15 mins	2	Prof Alessia Bacchi	1194
23-08-2017	1455-1730	MR 1.05	Special Activities	MS-032: Crystallography courses around the world	1877	Crystallography courses in Latin America	Oral 15 mins	3	Dr Diego Germán Lamas	1323

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23-08-2017	1455-1730	MR 1.05	Special Activities	MS-032: Crystallography courses around the world	1190	IUCr-UNESCO OpenLab: 25 editions in 22 countries and counting	Oral 15 mins	4	Dr Michele Zema	1493
23-08-2017	1455-1730	MR 1.05	Special Activities	MS-032: Crystallography courses around the world	1842	Crystallography at the Master level. MCC and beyond	Oral 15 mins	5	Dr Fermín Otálora	1870
23-08-2017	1455-1730	MR 1.05	Special Activities	MS-032: Crystallography courses around the world	1583	Expanding Crystallography as Science in Africa: Some Initiatives	Oral 15 mins	6	Prof Andreas Roodt	1739
23-08-2017	1455-1730	MR 1.05	Special Activities	MS-032: Crystallography courses around the world	219	FEBS practical crystallization courses since 2004	Oral 15 mins	7	Prof Ivana Kuta Smatanova	556
23-08-2017	1455-1730	MR 1.05	Special Activities	MS-032: Crystallography courses around the world	1915	Crystallography courses and industry: hand in hand across the land	Oral 15 mins	8	Dr Dubravka Sisak Jung	1322
23-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-033: Magnetic diffuse scattering and magnetic PDF analysis			CHAIR	0	Werner Schweika	1830
23-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-033: Magnetic diffuse scattering and magnetic PDF analysis			CHAIR	0	Branton Campbell	1928
23-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-033: Magnetic diffuse scattering and magnetic PDF analysis	80	Recent advances in the magnetic pair distribution function technique	Oral 30 mins	1	Dr Benjamin Allen Frandsen	282
23-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-033: Magnetic diffuse scattering and magnetic PDF analysis	1447	Emergent Order in the Frustrated Kagome Magnet Dy3Mg2Sb3O14	Oral 30 mins	2	Dr Joseph Paddison	1656
23-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-033: Magnetic diffuse scattering and magnetic PDF analysis	1171	Spiral spin-liquid and a vortex-like state in MnSc2S4	Oral 30 mins	3	Mr Shang Gao	1486
23-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-033: Magnetic diffuse scattering and magnetic PDF analysis	842	3D-magnetic difference-PDF analysis of magnetic frustration in Bixbyite	Oral 30 mins	4	Mr Nikolaj Roth	1230
23-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-034: Synthesis and properties of multi ferroics and multi-functional materials			CHAIR	0	Francesco Mezzadri	1925
23-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-034: Synthesis and properties of multi ferroics and multi-functional materials	306	Trirutiles as potential multiferroics: the case of Mn2TeO6	Oral 30 mins	1	Ms Nami Matsubara	705
23-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-034: Synthesis and properties of multi ferroics and multi-functional materials	1888	Incommensurate Magnetic Structure and Chemical Modulation in SbVO4 Catalyst	Oral 30 mins	2	Dr Jorge Hernández-Velasco	1973

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23-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-034: Synthesis and properties of multi ferroics and multi-functional materials	1884	H- bonded supramolecular ferroelectric materials supported by organoamino phosphonium cations	Oral 30 mins	3	Mr T Vijayakanth	1854
23-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-034: Synthesis and properties of multi ferroics and multi-functional materials	1088	Structural and magnetoelectric effect of $(x)\text{Li}_0.1\text{Cu}_0.1\text{Co}_0.1\text{Zn}_0.6\text{Fe}_2.1\text{O}_4 + (1-x)\text{Ba}_0.95\text{Ca}_0.05\text{TiO}_3$ multi	Oral 30 mins	4	Ms Roksana Parvin	1384
23-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-034: Synthesis and properties of multi ferroics and multi-functional materials	739	Crystal structure and ferroelectric properties of $(1-x)\text{Na}_0.5\text{Bi}_0.5\text{TiO}_3 - x\text{BaTiO}_3$ ceramics	Oral 30 mins	5	Dr Dillip K. Pradhan	719
23-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-035: Crystal structure relationships and their applications			CHAIR	0	Wolfgang Schmahl	2176
23-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-035: Crystal structure relationships and their applications			CHAIR	0	V. M. Talanov	207
23-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-035: Crystal structure relationships and their applications	498	Applications of the superspace concept in crystal chemistry	Oral 30 mins	1	Prof Gervais Chapuis	129
23-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-035: Crystal structure relationships and their applications	1220	Information-based measures of structural complexity of crystals	Oral 30 mins	2	Prof Sergey V. Krivovichev	1527
23-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-035: Crystal structure relationships and their applications	1797	Algebraic search for cooperative-rotational rigid-unit modes	Oral 30 mins	3	Prof Branton Campbell	1928
23-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-035: Crystal structure relationships and their applications	1029	Antiferrodistortive Isostructural Phase Transition in Perovskites	Oral 30 mins	4	Prof Dhananjai Pandey	1365
23-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-035: Crystal structure relationships and their applications	1849	Bond softness-sensitive bond valence parameters for crystal structure plausibility tests	Oral 15 mins	5	Prof Stefan Adams	1971
23-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-035: Crystal structure relationships and their applications	1209	New insights into the bonding mechanism of boron carbide	Oral 15 mins	6	Dr Swastik Mondal	1508

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23-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-036: Structural immunology and receptor signalling			CHAIR	0	Mike Lawrence	2026
23-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-036: Structural immunology and receptor signalling			CHAIR	0	Yvonne Jones	153
23-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-036: Structural immunology and receptor signalling	976	Broad neutralization of Influenza virus and implications for universal therapies	Oral 30 mins	1	Prof Ian Andrew Wilson	581
23-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-036: Structural immunology and receptor signalling	1966	T cell receptors have some more tricks up their sleeves.	Oral 30 mins	2	Dr Stephanie Gras	2120
23-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-036: Structural immunology and receptor signalling	195	Clustered protocadherin molecular assembly and implications for neuronal self-avoidance	Oral 30 mins	3	Dr Kerry Marie Goodman	529
23-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-036: Structural immunology and receptor signalling	947	How ligand binds to the insulin-like growth factor receptor	Oral 30 mins	4	Dr Yibin Xu	890
23-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-036: Structural immunology and receptor signalling	232	Structural insights into the signaling of the human Interleukin-3 receptor	Oral 15 mins	5	Prof Michael William Parker	101
23-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-036: Structural immunology and receptor signalling	981	Structural basis of Zika virus neutralization by highly potent antibody	Oral 15 mins	6	Dr Arvind Sharma	695
24-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-037: Macromolecular structures by hybrid methods			CHAIR	0	Jill Trehwella	144
24-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-037: Macromolecular structures by hybrid methods			CHAIR	0	Amit Sharma	150
24-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-037: Macromolecular structures by hybrid methods	1965	Structural Approaches to understanding Influenza Virus replication and transcription	Oral 30 mins	1	Prof Jonathan Grimes	696
24-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-037: Macromolecular structures by hybrid methods	307	Small-angle neutron scattering for the study of biomacromolecular complexes	Oral 30 mins	2	Dr Frank Richard Gabel	707
24-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-037: Macromolecular structures by hybrid methods	252	Structural basis for an autoubiquitination-targeted lysine by E2-E3 complex	Oral 30 mins	3	Dr Madhanagopal Anandapadamana ban	625



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24-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-037: Macromolecular structures by hybrid methods	345	Structural studies of dynamic CD4 changes relevant to HIV infection	Oral 30 mins	4	Ms Jennifer Anne Channell	545
24-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-037: Macromolecular structures by hybrid methods	478	Structural characterization of pseudo-dihydroorotase domain in yeast URA2	Oral 15 mins	5	Ms Yujung Jeon	679
24-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-037: Macromolecular structures by hybrid methods	1370	A Data Dictionary For Archiving Integrative/Hybrid Models	Oral 15 mins	6	Dr Brinda Vallat	1619
24-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-038: Porous framework materials for separation			CHAIR	0	Jie-Peng Zhang	373
24-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-038: Porous framework materials for separation			CHAIR	0	Satoshi Horike	500
24-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-038: Porous framework materials for separation	108	Metal Organic Frameworks Energy and Environmental Applications	Oral 30 mins	1	Dr Praveen Kumar THALLAPALLY	358
24-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-038: Porous framework materials for separation	171	Lanthanide Metal-Organic Frameworks: Synthesis and Applications	Oral 30 mins	2	Dr Wei Shi	488
24-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-038: Porous framework materials for separation	417	Targeted Synthesis of Porous Aromatic Frameworks	Oral 30 mins	3	Prof Guangshan Zhu	824
24-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-038: Porous framework materials for separation	1960	Mechanical Alloying of MOFs and Selective Capture of 1,3-Butadiene	Oral 30 mins	4	Dr Satoshi Horike	500
24-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-038: Porous framework materials for separation	152	Covalent Organic Framework Thin-Films For Molecular Separation	Oral 15 mins	5	Mr Kaushik Dey	235
24-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-038: Porous framework materials for separation	504	Computational Exploration of Interesting Gas Adsorption/Separation in MOFs	Oral 15 mins	6	Dr Renjith S. Pillai	913
24-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-039: Structural chemistry in 2-D: Crystal growth, surface structure and morphology			CHAIR	0	Matthew Hill	2387
24-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-039: Structural chemistry in 2-D: Crystal growth, surface structure and morphology	2083	Recent Adventures with Porous Materials: Triggered Release and Anti-aging Membranes	Oral 30 mins	1	Prof Matthew Hill	2387
24-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-039: Structural chemistry in 2-D: Crystal growth, surface structure and morphology	1650	3D Reciprocal Space Maps measurements for ultrathin polycrystalline materials	Oral 30 mins	2	Dr Jayanth Channagiri	1229

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24-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-039: Structural chemistry in 2-D: Crystal growth, surface structure and morphology	115	Metal-organic framework as efficient electrocatalyst for oxygen evolution reaction	Oral 30 mins	3	Prof Jie-Peng Zhang	373
24-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-039: Structural chemistry in 2-D: Crystal growth, surface structure and morphology	68	Decoding the Morphological Diversity in Two Dimensional Crystalline Porous Polymers	Oral 30 mins	4	Mr Arjun Halder	222
24-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-040: Microstructure, defects, stress and strain determination and modelling with powder diffraction data			CHAIR	0	Takashi Ida	1069
24-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-040: Microstructure, defects, stress and strain determination and modelling with powder diffraction data			CHAIR	0	Davor Balzar	295
24-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-040: Microstructure, defects, stress and strain determination and modelling with powder diffraction data	1463	Temperature Evolution of Microstructure of Deformed Submicrocrystalline Cu-Zr samples	Oral 30 mins	1	Prof Radomir Kuzel	530
24-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-040: Microstructure, defects, stress and strain determination and modelling with powder diffraction data	838	High-temperature 3D-RSM, phase transition and stress relaxation in pure zirconia	Oral 30 mins	2	Prof Rene Guinebretiere	1223
24-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-040: Microstructure, defects, stress and strain determination and modelling with powder diffraction data	493	Study of multilayer microstructure by XRD using noncoplanar measurement geometry	Oral 30 mins	3	Prof Alexander Ulyanekov	902
24-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-040: Microstructure, defects, stress and strain determination and modelling with powder diffraction data	165	Powder X-ray diffraction applications with single crystal diffractometers	Oral 30 mins	4	Dr Bob He	485
24-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-040: Microstructure, defects, stress and strain determination and modelling with powder diffraction data	832	Resonant diffraction study of structural disorder in Nb3Sn	Oral 15 mins	5	Mr Roman Svetogorov	1217

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24-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-040: Microstructure, defects, stress and strain determination and modelling with powder diffraction data	1232	An approach to identify the atomic arrangement in nanometer range-size	Oral 15 mins	6	Mr Hantaro Ozawa	1387
24-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-041: Advances in computational methods for powder diffraction			CHAIR	0	Basab Chattopadhyay	305
24-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-041: Advances in computational methods for powder diffraction			CHAIR	0	Andy Fitch	542
24-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-041: Advances in computational methods for powder diffraction	247	TOPAS – Programming Ideas	Oral 30 mins	1	Dr Alan Anthony Coelho	559
24-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-041: Advances in computational methods for powder diffraction	187	Crystal structure solution from thin films: software requirements	Oral 30 mins	2	Prof Roland Resel	518
24-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-041: Advances in computational methods for powder diffraction	1549	Exhaustive Symmetry Mode Searches: Phase Transitions in Pyrochlore Bi <sub>2</sub> Sn <sub>2</sub> O <sub>7</sub>	Oral 30 mins	3	Dr Eric Reinheimer	2541
24-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-041: Advances in computational methods for powder diffraction	939	Modern machine learning tools for crystallography	Oral 30 mins	4	Dr Paolo Bosetti	1294
24-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-041: Advances in computational methods for powder diffraction	1405	New refinement approach for crystal structure analysis of organic compounds	Oral 15 mins	5	Dr Akito Sasaki	1640
24-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-041: Advances in computational methods for powder diffraction	272	Imaging of Crystalline regions in Cotton fibers using Powder XRD	Oral 15 mins	6	Mr Manju V V	664
24-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-042: High-resolution spectroscopy			CHAIR	0	Dimosthenis Sokaras	2050
24-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-042: High-resolution spectroscopy			CHAIR	0	Dennis Nordlund	2123
24-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-042: High-resolution spectroscopy	1332	Predictive Modeling of Resonant Inelastic X-ray Scattering with OCEAN	Oral 30 mins	1	Dr John Thomas Vinson	1587
24-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-042: High-resolution spectroscopy	1138	X-ray Raman scattering spectroscopy at the ESRF	Oral 30 mins	2	Dr Christoph J. Sahle	1454
24-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-042: High-resolution spectroscopy	1665	The Endstation "NanoPES" at the Kurchatov synchrotron radiation source	Oral 30 mins	3	Mr Ratibor Chumakov	1817

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24-08-2017	1030-1305	MR 2.01	Physical and/or Fundamental	MS-043: Models for refining the electron density from elastic scattering. Bob Stewart's legacy			CHAIR	0	T. N. Guru Row	494
24-08-2017	1030-1305	MR 2.01	Physical and/or Fundamental	MS-043: Models for refining the electron density from elastic scattering. Bob Stewart's legacy			CHAIR	0	Paulina Dominiak	532
24-08-2017	1030-1305	MR 2.01	Physical and/or Fundamental	MS-043: Models for refining the electron density from elastic scattering. Bob Stewart's legacy	392	Development and application of X-ray quantum crystallographic methods	Oral 30 mins	1	Prof Simon Grabowsky	570
24-08-2017	1030-1305	MR 2.01	Physical and/or Fundamental	MS-043: Models for refining the electron density from elastic scattering. Bob Stewart's legacy	515	Advanced tools for charge density refinement and estimation of errors	Oral 30 mins	2	Dr Christian Jelsch	928
24-08-2017	1030-1305	MR 2.01	Physical and/or Fundamental	MS-043: Models for refining the electron density from elastic scattering. Bob Stewart's legacy	983	MO determination from experimental X-ray structure factors of diformohydrazide	Oral 30 mins	3	Prof Kiyooki Tanaka	1329
24-08-2017	1030-1305	MR 2.01	Physical and/or Fundamental	MS-043: Models for refining the electron density from elastic scattering. Bob Stewart's legacy	1508	Waverfunction refinement derived spin density of two cAAC-SiCl <sub>3</sub> polymorphs	Oral 30 mins	4	Dr Birger Dittrich	1689
24-08-2017	1030-1305	MR 2.01	Physical and/or Fundamental	MS-043: Models for refining the electron density from elastic scattering. Bob Stewart's legacy	932	Core electron deformation in silicon from powder X-ray diffraction	Oral 15 mins	5	Mr Kasper Tolborg	1281
24-08-2017	1030-1305	MR 2.01	Physical and/or Fundamental	MS-043: Models for refining the electron density from elastic scattering. Bob Stewart's legacy	1481	Topological analysis of hydrogen bonds and interaction energies in proteins	Oral 15 mins	6	Mr Suman Kumar Mandal	395
24-08-2017	1030-1305	MR 2.02	Special Activities	MS-044: Structural databases as teaching tools - Part A (macromolecules)			CHAIR	0	Joel Sussman	2015

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24-08-2017	1030-1305	MR 2.02	Special Activities	MS-044: Structural databases as teaching tools - Part A (macromolecules)			CHAIR	0	Christine Zardecki	1614
24-08-2017	1030-1305	MR 2.02	Special Activities	MS-044: Structural databases as teaching tools - Part A (macromolecules)	1969	Enlightening macromolecular structure-function relationship with Proteopedia	Oral 30 mins	1	Prof Jaime Prilusky	332
24-08-2017	1030-1305	MR 2.02	Special Activities	MS-044: Structural databases as teaching tools - Part A (macromolecules)	657	Structural view of biology: Exploring new perspectives for deeper learning	Oral 30 mins	2	Dr Shuchisimta Dutta	1073
24-08-2017	1030-1305	MR 2.02	Special Activities	MS-044: Structural databases as teaching tools - Part A (macromolecules)	1996	Disease to therapeutics via 3D structures: stories from viral world	Oral 30 mins	3	Dr Urmila Kulkarni-Kale	2173
24-08-2017	1030-1305	MR 2.02	Special Activities	MS-044: Structural databases as teaching tools - Part A (macromolecules)	631	PDBe: Bringing structure to biology and beyond	Oral 30 mins	4	Dr Matthew J Conroy	1050
24-08-2017	1030-1305	MR 2.02	Special Activities	MS-044: Structural databases as teaching tools - Part A (macromolecules)	1304	SASBDB and DARA as biological solution scattering teaching tools	Oral 15 mins	5	Dr Alexey Kikhney	509
24-08-2017	1030-1305	MR 2.02	Special Activities	MS-044: Structural databases as teaching tools - Part A (macromolecules)	1997	Play with 3D structure data of biomolecules - PDBj	Oral 15 mins	6	Dr Hirofumi Suzuki	2175

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24-08-2017	1030-1305	MR 2.03-2.04	Special Activities	MS-045: Structural data bases as teaching tools - Part B (organics, minerals)			CHAIR	0	Amy Sarjeant	171
24-08-2017	1030-1305	MR 2.03-2.04	Special Activities	MS-045: Structural data bases as teaching tools - Part B (organics, minerals)			CHAIR	0	Graciela Delgado	611
24-08-2017	1030-1305	MR 2.03-2.04	Special Activities	MS-045: Structural data bases as teaching tools - Part B (organics, minerals)	624	Teaching Undergraduates about Structure Using Database Examples	Oral 30 mins	1	Prof Louise Nicole Dawe	1043
24-08-2017	1030-1305	MR 2.03-2.04	Special Activities	MS-045: Structural data bases as teaching tools - Part B (organics, minerals)	1274	Crystallography as an introduction to Cheminformatics	Oral 30 mins	2	Prof Simon John Coles	312
24-08-2017	1030-1305	MR 2.03-2.04	Special Activities	MS-045: Structural data bases as teaching tools - Part B (organics, minerals)	648	Teaching Crystallography using the Powder Diffraction File	Oral 30 mins	3	Prof José Miguel Delgado	989
24-08-2017	1030-1305	MR 2.03-2.04	Special Activities	MS-045: Structural data bases as teaching tools - Part B (organics, minerals)	1002	Representation of physical properties in the material properties open database	Oral 30 mins	4	Mr Edgar Eduardo Villalobos	1337
24-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-046: Macromolecular structure determination at XFEL sources			CHAIR	0	Arwen Pearson	904
24-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-046: Macromolecular structure determination at XFEL sources			CHAIR	0	Makina Yabashi	2032
24-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-046: Macromolecular structure determination at XFEL sources	1610	X-ray Crystallography and Spectroscopy of Metalloenzymes Using Drop-on-Tape Method	Oral 30 mins	1	Dr Junko Yano	1760
24-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-046: Macromolecular structure determination at XFEL sources	425	A molecular movie of structural changes in bacteriorhodopsin	Oral 30 mins	2	Dr Eriko Nango	830
24-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-046: Macromolecular structure determination at XFEL sources	1151	Virus structures recovered from correlations in scattered XFEL pulses	Oral 30 mins	3	Dr Ruslan Kurta	1259
24-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-046: Macromolecular structure determination at XFEL sources	1309	On-Demand Acoustic Methods for Time-Resolved Structural Biology	Oral 30 mins	4	Dr Allen Milster Orville	1570

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24-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-046: Macromolecular structure determination at XFEL sources	622	Versatile and efficient rapid-mixing liquid jets	Oral 15 mins	5	Dr Diana CF Monteiro	1042
24-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-046: Macromolecular structure determination at XFEL sources	940	Serial synchrotron crystallography at EMBL PETRA III beamline P14.	Oral 15 mins	6	Dr Johanna Hakanpää	1295
24-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-047: Crystalline materials characterization with combined techniques			CHAIR	0	Koen Janssens	1168
24-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-047: Crystalline materials characterization with combined techniques			CHAIR	0	Alejandro Ayala	80
24-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-047: Crystalline materials characterization with combined techniques	513	On site analysis of paintings by using portable instruments	Oral 30 mins	1	Prof Izumi Nakai	927
24-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-047: Crystalline materials characterization with combined techniques	1525	Getting More for Less: Adaptive X-ray Fluorescence Sampling for Imaging	Oral 30 mins	2	Prof Marc Walton	1703
24-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-047: Crystalline materials characterization with combined techniques	1519	Combining characterization techniques at the NSLS-II	Oral 30 mins	3	Mr Eric Dooryhee	1701
24-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-047: Crystalline materials characterization with combined techniques	774	Disordered zeolite solved by combining electron diffraction, HRTEM and XRPD	Oral 15 mins	4	Ms Magdalena Ola Cichocka	834
24-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-047: Crystalline materials characterization with combined techniques	107	Crystallochemical characterization of polyoxometalate new minerals	Oral 15 mins	5	Dr Marcelo B Andrade	357
24-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-047: Crystalline materials characterization with combined techniques	1921	TAILORING MOLECULAR MULTIFERROIC COMPOUNDS: NEUTRON STUDIES ON FORMATE FRAMEWORKS	Oral 15 mins	6	Dr Laura Cañadillas-Delgado	2022
24-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-047: Crystalline materials characterization with combined techniques	26	Scanning transmission electron microscopy assessment of a metal-organic framework compound	Oral 15 mins	7	Prof Peter Moeck	78

Date	Time	Hall	Theme	Microsymposium (MS)	ABS-Num.	Abstract Title	Presentation Type	Sequence	Chair/Author Name	Database ID
24-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-048: Supramolecular synthons at the confluence of theory and practice			CHAIR	0	P Venugopalan	431
24-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-048: Supramolecular synthons at the confluence of theory and practice			CHAIR	0	Catharine Esterhuysen	841
24-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-048: Supramolecular synthons at the confluence of theory and practice	1563	Hydrogen Bonds and Halogen Bonds: Solid-State, Solution-Phase and Theory	Oral 30 mins	1	Prof Lee Brammer	1729
24-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-048: Supramolecular synthons at the confluence of theory and practice	1047	Molecules to Materials: Supramolecular Synthons and 2D Metal-Organic Nanosheets	Oral 30 mins	2	Prof Narasimha Moorthy Jarugu	1130
24-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-048: Supramolecular synthons at the confluence of theory and practice	557	Guest exchange and guest influence in dynamic frameworks	Oral 30 mins	3	Prof Susan Ann Bourne	973
24-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-048: Supramolecular synthons at the confluence of theory and practice	1004	Identifying non-conventional supramolecular synthons in the crystalline state	Oral 30 mins	4	Prof Edward R.T. Tiekink	135
24-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-048: Supramolecular synthons at the confluence of theory and practice	1205	Chiral H-bonded chains: a key to non-centrosymmetric co-crystals of 3,5-dinitropyridine-2(1H)-one	Oral 15 mins	5	Dr Ivan Fedyanin	1264
24-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-048: Supramolecular synthons at the confluence of theory and practice	753	Bond-valence vector model in analysis of boron coordination sphere	Oral 15 mins	6	Dr Izabela D. Madura	1158



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24-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-049: In-situ and in-operando characterization of catalytic and functional materials			CHAIR	0	Antonio F. Moreira Dos Santos	1344
24-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-049: In-situ and in-operando characterization of catalytic and functional materials			CHAIR	0	Miguel Delgado	989
24-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-049: In-situ and in-operando characterization of catalytic and functional materials	894	Correlating the chronology and local structure of energy materials	Oral 30 mins	1	Dr Daniel Olds	1270
24-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-049: In-situ and in-operando characterization of catalytic and functional materials	452	Development of operando Techniques for Battery Study using SPICA	Oral 30 mins	2	Dr Masao Yonemura	849
24-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-049: In-situ and in-operando characterization of catalytic and functional materials	1672	In situ synthesis and reduction of functional sulfides	Oral 30 mins	3	Prof Daniel Shoemaker	1823
24-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-049: In-situ and in-operando characterization of catalytic and functional materials	1509	New Techniques to Determine Structural Transformations of Active Catalysts	Oral 30 mins	4	Dr Jonathan Hanson	1691
24-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-049: In-situ and in-operando characterization of catalytic and functional materials	1095	In situ XRD study of Mn-containing oxide catalysts	Oral 30 mins	5	Olga Bulavchenko	1094

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24-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-050: Small-Angle Scattering studies of biomacromolecular kinetics			CHAIR	0	Pau Bernado	504
24-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-050: Small-Angle Scattering studies of biomacromolecular kinetics			CHAIR	0	Clement Blanchet	1182
24-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-050: Small-Angle Scattering studies of biomacromolecular kinetics	683	Structural Exploring Multi-component Equilibrium in Biological Systems	Oral 30 mins	1	Prof Hironari Kamikubo	1092
24-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-050: Small-Angle Scattering studies of biomacromolecular kinetics	1579	Combined SAXS and Microfluidics for time-resolved structural studies of bimolecules	Oral 30 mins	2	Prof Lise Arleth	1738
24-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-050: Small-Angle Scattering studies of biomacromolecular kinetics	494	High-throughput BioSAXS at ESRF BM29	Oral 30 mins	3	Dr Martha Elisabeth Brennich	901
24-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-050: Small-Angle Scattering studies of biomacromolecular kinetics	1028	Coupling microfluidics and SAXS to study the whole crystallization process	Oral 30 mins	4	Dr Sébastien Teychené	1362
24-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-050: Small-Angle Scattering studies of biomacromolecular kinetics	740	High-flux time-resolved experiments and anomalous scattering at EMBL P12 beamline	Oral 15 mins	5	Dr Andrey Gruzinov	905
24-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-050: Small-Angle Scattering studies of biomacromolecular kinetics	1746	Synthetic polymers: WAXS and SAXS methods to understand materials functionality	Oral 15 mins	6	Dr Antonia Neels	1884
24-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-051: Recent developments in XAFS spectroscopy: Theory, instrumentation and data analysis			CHAIR	0	Konstantin Klementiev	1861
24-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-051: Recent developments in XAFS spectroscopy: Theory, instrumentation and data analysis	1818	EXAFS at the future diffraction limited storage ring PETRA IV	Oral 30 mins	1	Dr Edmund Welter	1803

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24-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-051: Recent developments in XAFS spectroscopy: Theory, instrumentation and data analysis	663	Novel Plasmon-Coupling Theory for XAFS and diffraction	Oral 30 mins	2	Prof Christopher Thomas Chantler	1079
24-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-051: Recent developments in XAFS spectroscopy: Theory, instrumentation and data analysis	1133	FPMS code with an interface to Electronic Structure codes	Oral 30 mins	3	Dr Keisuke Hatada	1432
24-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-051: Recent developments in XAFS spectroscopy: Theory, instrumentation and data analysis	716	Creating a robust,extensible XAS data standard	Oral 30 mins	4	Dr James Reginald Hester	1121
24-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-051: Recent developments in XAFS spectroscopy: Theory, instrumentation and data analysis	1988	ParSeq: parallel execution of sequential data analysis applied to XAFS	Oral 15 mins	5	Dr Konstantin Klementiev	1861
24-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-051: Recent developments in XAFS spectroscopy: Theory, instrumentation and data analysis	668	XAFS, Fluorescence, XANES, RIXS, XERT data formats and coding	Oral 15 mins	6	Prof Christopher Thomas Chantler	1079
24-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-052: Minerals/gems in industrial applications			CHAIR	0	Patrick Mercier	1003
24-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-052: Minerals/gems in industrial applications			CHAIR	0	Fermin Otorala	1870
24-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-052: Minerals/gems in industrial applications	265	Biomimetic citrate-coated nanopatites for biomedical and industrial applications	Oral 30 mins	1	Dr Jaime Gomez Morales	646
24-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-052: Minerals/gems in industrial applications	818	Accuracy in Quantitative Phase Analysis: The Impact of Instrument Geometry	Oral 30 mins	2	Dr Matthew Ryan Rowles	897
24-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-052: Minerals/gems in industrial applications	353	Polytypism in Natural SiC Using Laue Microdiffraction at ALS 12.3.2	Oral 30 mins	3	Dr Camelia Veronica Stan	762
24-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-052: Minerals/gems in industrial applications	821	Synthesis and Characterization of Multifunctional Mineral Beyerite (CaBi2O2(CO3)2)	Oral 30 mins	4	Ms Meenakshi Pokhriyal	1210

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24-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-052: Minerals/gems in industrial applications	1876	Iron oxide for arsenic removal in water: synthesis and characterization	Oral 15 mins	5	Dr Luis Guillermo Romero-Esquivel	1990
24-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-052: Minerals/gems in industrial applications	1722	Local structures of Ca, Ti, Fe in shergottite fusion glass	Oral 15 mins	6	Mr Tsubasa Tobase	1864
24-08-2017	1455-1730	MR 2.02	Special Activities	MS-053: Scientific value of raw data			CHAIR	0	Loes Kroon-Batenburg	398
24-08-2017	1455-1730	MR 2.02	Special Activities	MS-053: Scientific value of raw data			CHAIR	0	Brian McMahon	1283
24-08-2017	1455-1730	MR 2.02	Special Activities	MS-053: Scientific value of raw data	584	Past and Future Uses of Raw Diffraction Data	Oral 30 mins	1	Prof George Phillips	2438
24-08-2017	1455-1730	MR 2.02	Special Activities	MS-053: Scientific value of raw data	1764	A Public Database of Macromolecular Diffraction Experiments	Oral 30 mins	2	Dr Marek Piotr Grabowski	1894
24-08-2017	1455-1730	MR 2.02	Special Activities	MS-053: Scientific value of raw data	1197	Treatment of X-ray Diffraction Data at Diamond Light Source	Oral 30 mins	3	Mr James Parkhurst	1450
24-08-2017	1455-1730	MR 2.02	Special Activities	MS-053: Scientific value of raw data	664	To merge or not to merge; to spline or ...	Oral 30 mins	4	Prof Christopher Thomas Chantler	1079
24-08-2017	1455-1730	MR 2.02	Special Activities	MS-053: Scientific value of raw data	1590	Macromolecular diffraction data fit for archiving	Oral 15 mins	5	Dr Andreas Foerster	1364
24-08-2017	1455-1730	MR 2.02	Special Activities	MS-053: Scientific value of raw data	1762	Crystallographic metadata from a front end perspective	Oral 15 mins	6	Dr Kamil Filip Dziubek	1549
24-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-054: Mechanisms of bacterial resistance			CHAIR	0	Natalie Strynadka	1605
24-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-054: Mechanisms of bacterial resistance			CHAIR	0	Miquel Coll	83
24-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-054: Mechanisms of bacterial resistance	1575	Structural studies of clinical resistomes	Oral 30 mins	1	Prof Albert Marinus Berghuis	1735
24-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-054: Mechanisms of bacterial resistance	2005	Studies of prokaryotic Type II topoisomerase drug inhibition	Oral 30 mins	2	Dr Mark Rutherford Sanderson	2151
24-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-054: Mechanisms of bacterial resistance	1354	Allosteric mechanism in PBP2a controlling resistance of Methicillin-resistant Staphylococcus aureus	Oral 30 mins	3	Prof Juan A. Hermoso	1543
24-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-054: Mechanisms of bacterial resistance	954	Structure and mechanistic insights into F/R1 plasmid conjugative relaxase	Oral 30 mins	4	Dr Aravindan Ilangovan	1313
24-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-054: Mechanisms of bacterial resistance	1530	Structural basis of nonhaemolytic nature of pneumolysin from strain ST-306	Oral 15 mins	5	Dr Dilip Badgujar	1639

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24-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-054: Mechanisms of bacterial resistance	1822	Crystal structure of an antigenic outer-membrane protein from Salmonella Typhi	Oral 15 mins	6	Prof Chun-Jung Chen	1951
25-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-055: New challenges in interpretation of structural data			CHAIR	0	Kurt Krause	898
25-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-055: New challenges in interpretation of structural data			CHAIR	0	George Phillips	2438
25-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-055: New challenges in interpretation of structural data	1984	Cryo-EM in the age of X-ray crystallography	Oral 30 mins	1	Prof Matthias Wolf	2158
25-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-055: New challenges in interpretation of structural data	1979	Artificial synthesis of supramolecular protein structures	Oral 30 mins	2	Dr Lawrence Kwong Ynyr Lee	2142
25-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-055: New challenges in interpretation of structural data	1698	How to solve, refine, validate, and deposit difficult macromolecular structures	Oral 15 mins	3	Dr Dominika Borek	1342
25-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-055: New challenges in interpretation of structural data	1214	Conquering non-isomorphism	Oral 15 mins	4	Prof Kay Diederichs	1413
25-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-055: New challenges in interpretation of structural data	1139	Online automated structure solution from multiple datasets	Oral 15 mins	5	Dr Santosh Panjekar	1066
25-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-055: New challenges in interpretation of structural data	1128	A novel method in modelling diffuse scattering in protein crystallography	Oral 15 mins	6	Mr Tim De Klijn	1451
25-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-055: New challenges in interpretation of structural data	896	Refinement of Macromolecular Structures at Low Resolution	Oral 15 mins	7	Dr Oleg Kovalevskiy	1257

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25-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-056: Direct observation of reactions and labile species within porous frameworks			CHAIR	0	Kumar Biradha	118
25-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-056: Direct observation of reactions and labile species within porous frameworks			CHAIR	0	Javier Rujas	1814
25-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-056: Direct observation of reactions and labile species within porous frameworks	656	Chemistry of Labile Small Sulfur Allotropes in Interactive Coordination Networks	Oral 30 mins	1	Dr Hiroyoshi Ohtsu	280
25-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-056: Direct observation of reactions and labile species within porous frameworks	878	Hybrid Halogen Bonded Frameworks: Topology Variety and Molecule Sorption Properties.	Oral 30 mins	2	Prof Giancarlo Terraneo	1123
25-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-056: Direct observation of reactions and labile species within porous frameworks	1639	Open Channels in Porous Molecular Crystals: Host-Guest Structures and Interactions	Oral 30 mins	3	Dr Hidehiro Uekusa	1517
25-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-056: Direct observation of reactions and labile species within porous frameworks	300	Chiral crystalline sponges: absolute structure determination of chiral guests	Oral 30 mins	4	Dr Ritesh Dubey	56
25-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-056: Direct observation of reactions and labile species within porous frameworks	22	Coordinative alignment of molecules in chiral metal-organic frameworks	Oral 15 mins	5	Dr Eugene Kapustin	55
25-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-056: Direct observation of reactions and labile species within porous frameworks	1387	Structural diversity of Coordination Polymers derived from Imidazole based Ligands	Oral 15 mins	6	Dr Anantharaman Ganapathi	1632
25-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-057: Charge density studies in crystal and cocrystal engineering			CHAIR	0	Tejender Thakur	82
25-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-057: Charge density studies in crystal and cocrystal engineering			CHAIR	0	Anna Krawczuk	1046
25-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-057: Charge density studies in crystal and cocrystal engineering	535	Localization-Delocalization Matrices: Bridging QTAIM and Chemical Graph Theory	Oral 30 mins	1	Prof Chérif Matta	947

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25-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-057: Charge density studies in crystal and cocrystal engineering	254	Cocrystal vs. Salt: Effect of crystal environment on molecular interactions	Oral 30 mins	2	Prof Enrique Espinosa	335
25-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-057: Charge density studies in crystal and cocrystal engineering	518	Using electron density to understand cocrystal structures	Oral 30 mins	3	Dr Julia Contreras-Garcia	931
25-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-057: Charge density studies in crystal and cocrystal engineering	1281	Using charge density to understand structure-property relationships in pharmaceutical co-crystals	Oral 30 mins	4	Prof Simon John Coles	312
25-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-057: Charge density studies in crystal and cocrystal engineering	1310	Efficient organic NLO material: Charge density analysis and device fabrication	Oral 15 mins	5	Mr Kunal Kumar Jha	75
25-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-057: Charge density studies in crystal and cocrystal engineering	1667	Cluster analysis of functional group polarizabilities	Oral 15 mins	6	Ms Michelle Ernst	1820

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25-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-058: Powder diffraction & polymorphism. Search, phase transformations and new polymorph identification			CHAIR	0	Anant Paradkar	1976
25-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-058: Powder diffraction & polymorphism. Search, phase transformations and new polymorph identification			CHAIR	0	Alan Goldman	158
25-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-058: Powder diffraction & polymorphism. Search, phase transformations and new polymorph identification	1613	Applications of X-ray Powder Diffractometry in Preformulation and Formulation Studies	Oral 30 mins	1	Prof Raj Suryanarayanan	1762
25-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-058: Powder diffraction & polymorphism. Search, phase transformations and new polymorph identification	1097	Quantitative phase analysis of polymorphs using only observed integrated intensities	Oral 30 mins	2	Dr Hideo Toraya	1425
25-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-058: Powder diffraction & polymorphism. Search, phase transformations and new polymorph identification	971	Adenine phase transformations in situ: crystalline, non-crystalline and in between	Oral 15 mins	3	Dr Dubravka Sisak Jung	1322
25-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-058: Powder diffraction & polymorphism. Search, phase transformations and new polymorph identification	1311	ICDD Full Diffraction Pattern Polymer Project for Biomedical Materials Characterization	Oral 30 mins	4	Dr Thomas Nelson Blanton	1577
25-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-058: Powder diffraction & polymorphism. Search, phase transformations and new polymorph identification	1717	Designed crystallization via sublimation	Oral 15 mins	5	Dr Sudarshan Mahapatra	1859



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25-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-058: Powder diffraction & polymorphism. Search, phase transformations and new polymorph identification	1077	Anomalous thermal behaviour and diffuse scattering in cadmium cyanide	Oral 15 mins	6	Ms Chloe Simone Coates	1407
25-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-058: Powder diffraction & polymorphism. Search, phase transformations and new polymorph identification	2108	PXRD and SSNMR Spectroscopy: Complimentary Techniques for Polymorph Identification	Oral 15 mins	7	Dr Eric Munson	2538

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25-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-059: Quantitative electron diffraction			CHAIR	0	Mauro Gemmi	1673
25-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-059: Quantitative electron diffraction			CHAIR	0	Enrico Mugnaioli	1449
25-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-059: Quantitative electron diffraction	447	Atomic structure of metal-ion battery cathodes with electron diffraction tomography	Oral 30 mins	1	Prof Artem Abakumov	838
25-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-059: Quantitative electron diffraction	1588	Dynamical refinement of modulated structures against electron diffraction data	Oral 30 mins	2	Dr Lukas Palatinus	1209
25-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-059: Quantitative electron diffraction	1974	Electron 3D crystallography of protein crystals for visualization of charges	Oral 30 mins	3	Dr Koji Yonekura	2132
25-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-059: Quantitative electron diffraction	1975	Locate light elements by electron diffraction	Oral 30 mins	4	Dr Junliang Sun	2136
25-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-059: Quantitative electron diffraction	325	Structure of the SnO <sub>2</sub> (110)-(4×1) with LEED I(E)	Oral 15 mins	5	Dr Katariina Pussi	728
25-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-059: Quantitative electron diffraction	751	Serial electron diffraction for phase analysis and structure determination	Oral 15 mins	6	Dr Stef Smeets	574
25-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-060: XAS at extreme conditions			CHAIR	0	Giuliana Aquilanti	1865
25-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-060: XAS at extreme conditions	409	EXAFS and laser-driven compression at the Omega and NIF facilities	Oral 30 mins	1	Dr Federica Coppari	816
25-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-060: XAS at extreme conditions	297	RIXS at extreme conditions at the GALAXIES beamline	Oral 30 mins	2	Dr Jean-Pascal Rueff	701
25-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-060: XAS at extreme conditions	448	Extreme condition beamline at SIRIUS to study rare-earths and actinides	Oral 30 mins	3	Dr Narcizo Marques De Souza Neto	848
25-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-060: XAS at extreme conditions	162	High pressure XRD and XAS Study of SnI <sub>4</sub>	Oral 30 mins	4	Dr Jean-Paul Itié	469

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25-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-061: Perovskites, perovskites and perovskites!			CHAIR	0	Maarit Karppinen	2006
25-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-061: Perovskites, perovskites and perovskites!			CHAIR	0	Prof. Venkataramanan Mahalingam	1812
25-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-061: Perovskites, perovskites and perovskites!	1475	Crystal/Magnetic Structures, Spin Correlations and Dynamics in Sr <sub>2</sub> YRuO <sub>6</sub> Double Perovskite	Oral 30 mins	1	Prof Eduardo Granado Monteiro Da Silva	1671
25-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-061: Perovskites, perovskites and perovskites!	241	Magnetic frustration and random exchange in double perovskites	Oral 30 mins	2	Dr Sami Vasala	481
25-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-061: Perovskites, perovskites and perovskites!	855	Polar and magnetic structures of NaLnCoWO <sub>6</sub> doubly ordered perovskites	Oral 30 mins	3	Dr Claire V. Colin	843
25-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-061: Perovskites, perovskites and perovskites!	1942	MULTIFERROELECTRICITY OF CORNER-SHARED PEROVSKITE NETWORKS OF MANGANESE AND OXYGEN	Oral 30 mins	4	Prof Omar Chmaissem	2081
25-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-061: Perovskites, perovskites and perovskites!	284	Insights on the structural transformations in NBT-xBT from polarized Raman	Oral 15 mins	5	Dr Gemma De La Flor Martin	521

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25-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-061: Perovskites, perovskites and perovskites!	458	Electric field induced monoclinic distortion and polarization rotation in Na <sub>0.5</sub> Bi <sub>0.5</sub> TiO <sub>3</sub>	Oral 15 mins	6	Dr Semën Gorfman	856
25-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-062: Topological magnetic structures : monopoles, skyrmions, etc.			CHAIR	0	Henrick Ronnow	2040
25-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-062: Topological magnetic structures : monopoles, skyrmions, etc.	1674	Complex mesoscale magnetic order in the Néel-type skyrmion material GaV <sub>4</sub> S <sub>8</sub>	Oral 30 mins	1	Dr Jonathan Stuart White	1828
25-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-062: Topological magnetic structures : monopoles, skyrmions, etc.	756	Structural and magnetic investigations of new skyrmion phases	Oral 30 mins	2	Prof Geetha Balakrishnan	992
25-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-062: Topological magnetic structures : monopoles, skyrmions, etc.	903	Magnetic frustration in rare earth zirconate pyrochlores	Oral 30 mins	3	Dr Monica Ciomaga Hatnean	1278
25-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-062: Topological magnetic structures : monopoles, skyrmions, etc.	2090	How Skyrmion Lattice Forms and Arranges	Oral 30 mins	4	Dr Ping Huang	2427
25-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-062: Topological magnetic structures : monopoles, skyrmions, etc.	2094	Magnetic quadrupolar order in the chiral square cupola compound BaTiOCu <sub>4</sub> (PO <sub>4</sub> ) <sub>4</sub>	Oral 30 mins	5	Henrick Ronnow	2040
25-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-063: Cell signalling, ubiquitination and cell death			CHAIR	0	Peter Czabotar	1067
25-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-063: Cell signalling, ubiquitination and cell death	1373	Signalling around DNA breaks – new tricks for old dogs!	Oral 30 mins	1	Dr Stephen John Smerdon	1621
25-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-063: Cell signalling, ubiquitination and cell death	1600	Regulation of RING ubiquitin ligases by small protein molecules	Oral 30 mins	2	Dr Danny Huang	1749
25-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-063: Cell signalling, ubiquitination and cell death	1978	How do MACPF/CDC pore forming protein punch holes in cells?	Oral 30 mins	3	Dr Michelle Dunstone	296

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25-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-063: Cell signalling, ubiquitination and cell death	1612	Regulation of WWP2 Ubiquitin Ligase	Oral 30 mins	4	Dr Sandra B. Gabelli	1761
25-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-063: Cell signalling, ubiquitination and cell death	1071	Structural Characterisation of SARM in Axon Degeneration and Cell Death	Oral 30 mins	5	Mr Shane Michael Horsefield	1400

Date	Time	Hall	Theme	Microsymposium (MS)	ABS-Num.	Abstract Title	Presentation Type	Sequence	Chair/Author Name	Database ID
25-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-064: Time and motion resolved imaging and diffraction			CHAIR	0	John Keith Moffat	2128
25-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-064: Time and motion resolved imaging and diffraction			CHAIR	0	Dominik Oberthuer	1016
25-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-064: Time and motion resolved imaging and diffraction	737	Time-resolved mixing-jet X-ray Free Electron Laser crystallography experiments	Oral 30 mins	1	Dr Dominik Oberthuer	1016
25-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-064: Time and motion resolved imaging and diffraction	822	Two colour imaging of ultrafast magnetisation dynamics	Oral 30 mins	2	Dr Clemens von Korff Schmising	1208
25-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-064: Time and motion resolved imaging and diffraction	1611	Room temperature femtosecond X-ray crystallography of Photosystem II	Oral 30 mins	3	Dr Jan Kern	1743
25-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-064: Time and motion resolved imaging and diffraction	2030	Femtosecond structural dynamics of trans/cis isomerization in photoactive yellow protein	Oral 30 mins	4	Dr Kanupriya Pande	2220
25-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-064: Time and motion resolved imaging and diffraction	475	BIMORPH X-RAY OPTICS FOR TIME-RESOLVED EXPERIMENTS	Oral 30 mins	5	Mr Anton Kulikov	870
25-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-065: New structures for natural and synthetic open framework materials			CHAIR	0	Florenzia Di Salvo	561
25-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-065: New structures for natural and synthetic open framework materials			CHAIR	0	Laszlo Fabian	2046
25-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-065: New structures for natural and synthetic open framework materials	1626	Minerals with Metal-Organic Framework Structures	Oral 30 mins	1	Prof Tomislav Friscic	1773
25-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-065: New structures for natural and synthetic open framework materials	806	Adding Flavours to our MOFs	Oral 30 mins	2	Prof Alessia Bacchi	1194
25-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-065: New structures for natural and synthetic open framework materials	274	Metal–Organic Frameworks with Multi-Components in Order	Oral 30 mins	3	Prof Qiaowei Li	665

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25-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-065: New structures for natural and synthetic open framework materials	735	Bismuth Coordination Polymers: From Centuries-old Medicines to Unprecedented Topological Complexity	Oral 30 mins	4	Dr Andrew Kentaro Inge	1141
25-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-065: New structures for natural and synthetic open framework materials	443	K <sub>2</sub> Ce(PO <sub>4</sub> ) <sub>2</sub> : A New Complex Phosphate of Ce(IV)	Oral 30 mins	5	Ms Samatha Bevara	71

Date	Time	Hall	Theme	Microsymposium (MS)	ABS-Num.	Abstract Title	Presentation Type	Sequence	Chair/Author Name	Database ID
25-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-066: Bending, jumping and rotating: Motion and movement in crystalline solids			CHAIR	0	C. Malla Reddy	122
25-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-066: Bending, jumping and rotating: Motion and movement in crystalline solids			CHAIR	0	Daisuke Hashizume	2028
25-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-066: Bending, jumping and rotating: Motion and movement in crystalline solids	685	Disintegrative vs Restorative Effects during Motion and Self-Healing of Crystals	Oral 30 mins	1	Prof Pance Naumov	1009
25-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-066: Bending, jumping and rotating: Motion and movement in crystalline solids	2000	Gold Isocyanide Complexes with Mechanical Response	Oral 30 mins	2	Prof Hajime Ito	2183
25-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-066: Bending, jumping and rotating: Motion and movement in crystalline solids	136	Crystal Jumping of Alkyl Acridone and its Dicyanomethylenated Derivatives	Oral 30 mins	3	Dr Takashi Takeda	430
25-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-066: Bending, jumping and rotating: Motion and movement in crystalline solids	94	Design of elastically bendable molecular crystals: Implications for smart actuators	Oral 15 mins	4	Dr Soumyajit Ghosh	319
25-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-066: Bending, jumping and rotating: Motion and movement in crystalline solids	1324	Quantitative approaches to crystal engineering: Applications to mechanical properties	Oral 15 mins	5	Dr Sajesh Pynadath Thomas	1586
25-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-066: Bending, jumping and rotating: Motion and movement in crystalline solids	350	Third Generation Crystal Engineering. Hand-Twisted Helical Crystals	Oral 15 mins	6	Mr Subhankar Saha	760
25-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-066: Bending, jumping and rotating: Motion and movement in crystalline solids	1914	Feedback mechanisms in single-crystal-to-single-crystal solid-state reactions	Oral 15 mins	7	Prof Manuel Antonio Fernandes	2016



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25-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-067: Grain mapping and spatially-resolved diffraction - reaching the ppm scale.			CHAIR	0	H. F. Poulsen	2371
25-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-067: Grain mapping and spatially-resolved diffraction - reaching the ppm scale.			CHAIR	0	Gavin Vaughan	2093
25-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-067: Grain mapping and spatially-resolved diffraction - reaching the ppm scale.	1932	Multi-scale 3D Characterization with Dark-Field X-Ray Microscopy	Oral 30 mins	1	Dr Hugh William Simons	2049
25-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-067: Grain mapping and spatially-resolved diffraction - reaching the ppm scale.	2017	Real-time chemical imaging of working catalytic membrane reactors	Oral 30 mins	2	Mr Antonios Vamvakeros	2211
25-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-067: Grain mapping and spatially-resolved diffraction - reaching the ppm scale.	862	Orientation mapping of steel by scanning three-dimensional x-ray diffraction microscopy	Oral 30 mins	3	Dr Yujiro Hayashi	1244
25-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-067: Grain mapping and spatially-resolved diffraction - reaching the ppm scale.	1030	Sub-millimetre-resolved X-ray phase analysis for materials science	Oral 30 mins	4	Dr Alexey Veligzhanin	1361
25-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-068: New X-ray sources: Storage rings - FELs- laser-based			CHAIR	0	Harald Reichert	2148
25-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-068: New X-ray sources: Storage rings - FELs- laser-based			CHAIR	0	Tetsuya Ishikawa	2084
25-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-068: New X-ray sources: Storage rings - FELs- laser-based	1881	Storage Ring X-ray Sources	Oral 30 mins	1	Prof Joel Donald Brock	1992
25-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-068: New X-ray sources: Storage rings - FELs- laser-based	2016	The European X-ray Free Electron Laser	Oral 30 mins	2	Prof Robert Feidenhansl	2209
25-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-068: New X-ray sources: Storage rings - FELs- laser-based	2013	Recent Progress of Laser-Driven Intense X-ray Sources and the Applications	Oral 30 mins	3	Dr Tetsuya Kawachi	2204
25-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-068: New X-ray sources: Storage rings - FELs- laser-based	1355	Structural Biology at the diffraction limited synchrotron source MAX IV	Oral 15 mins	4	Dr Marjolein Thunnissen	1607
25-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-068: New X-ray sources: Storage rings - FELs- laser-based	917	New dimensions for imaging and diffraction research at European XFEL	Oral 15 mins	5	Dr Alexander Blagov	1285

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25-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-068: New X-ray sources: Storage rings - FELs- laser-based	1581	Development of Automated Home-Lab Beamlines	Oral 15 mins	6	Dr Vernon Russell Smith	1737
25-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-068: New X-ray sources: Storage rings - FELs- laser-based	936	PHASE beamline at Kurchatov synchrotron light source.	Oral 15 mins	7	Dr Roman Senin	1274
25-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-069: High-pressure crystallography as the ultimate interdisciplinary tool			CHAIR	0	Dr Ines Collings	1254
25-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-069: High-pressure crystallography as the ultimate interdisciplinary tool			CHAIR	0	A. Goodwin	1534
25-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-069: High-pressure crystallography as the ultimate interdisciplinary tool	215	Reactivity of Elements and Compounds:Results of Structure Prediction AlgorithmUSPEX	Oral 30 mins	1	Prof Artem Oganov	550
25-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-069: High-pressure crystallography as the ultimate interdisciplinary tool	444	Triggering Dynamic Structural Changes in Lipid Membranes	Oral 30 mins	2	Dr Nicholas Jan Brooks	844
25-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-069: High-pressure crystallography as the ultimate interdisciplinary tool	1558	Novel Compounds synthesized at High Pressure-High Temperatures	Oral 30 mins	3	Dr Maddury Somayazulu	1722
25-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-069: High-pressure crystallography as the ultimate interdisciplinary tool	1276	Novel Modulated Structure of Superconducting Hydrogen Sulfide	Oral 30 mins	4	Prof John S Tse	1557
25-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-069: High-pressure crystallography as the ultimate interdisciplinary tool	510	High-Pressure X-ray Diffraction and Mössbauer Spectroscopy Study of Fe <sub>1.087</sub> Te	Oral 15 mins	5	Prof Jens-Erik Jørgensen	549
25-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-069: High-pressure crystallography as the ultimate interdisciplinary tool	243	Putting pressure on WOMBAT – outcomes and unique capabilities	Oral 15 mins	6	Dr Helen Elizabeth Maynard-Casely	514

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25-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-070: Superconducting materials			CHAIR	0	Irina Makarova	544
25-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-070: Superconducting materials			CHAIR	0	R. J. McQueeney	2121
25-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-070: Superconducting materials	627	Tc-enhancement of Fe1+ $\delta$ Se by electrochemical lithium intercalation	Oral 30 mins	1	Prof Evgeny Antipov	934
25-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-070: Superconducting materials	1239	The electron microscopy of superconducting materials	Oral 30 mins	2	Dr Alexander L Vasiliev	642
25-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-070: Superconducting materials	1971	Coexistence of superconductivity and ferromagnetism in Eu-based Fe pnictides	Oral 30 mins	3	Prof Shibabrata Nandi	2125
25-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-070: Superconducting materials	525	Lattice location of Ta and Ti in doped Nb3Sn	Oral 30 mins	4	Dr Steve Michael Heald	937
25-08-2017	1455-1730	MR 2.02	Special Activities	MS-071: Crystallographic patterns in art and cultural heritage			CHAIR	0	Louise De Las Penas	526
25-08-2017	1455-1730	MR 2.02	Special Activities	MS-071: Crystallographic patterns in art and cultural heritage			CHAIR	0	Rima Ajlouni	1340
25-08-2017	1455-1730	MR 2.02	Special Activities	MS-071: Crystallographic patterns in art and cultural heritage	114	The different tiling of 12-fold rosettes in Moroccan geometric art	Oral 30 mins	1	Prof Youssef Aboufadil	366
25-08-2017	1455-1730	MR 2.02	Special Activities	MS-071: Crystallographic patterns in art and cultural heritage	25	Quantitative classification of periodic gray-level patterns by geometric AIC	Oral 30 mins	2	Prof Peter Moeck	78
25-08-2017	1455-1730	MR 2.02	Special Activities	MS-071: Crystallographic patterns in art and cultural heritage	2074	Crystallographic Patterns in Philippine Indigenous Fabrics	Oral 30 mins	3	Prof Ma. Louise Antonette Delas Penas	526
25-08-2017	1455-1730	MR 2.02	Special Activities	MS-071: Crystallographic patterns in art and cultural heritage	2077	A generalized structural model for generating quasi-periodic formations	Oral 30 mins	4	Dr Rima Ajlouni	1340

Date	Time	Hall	Theme	Microsymposium (MS)	ABS-Num.	Abstract Title	Presentation Type	Sequence	Chair/Author Name	Database ID
25-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-072: Solving the phase problem without experimental phasing			CHAIR	0	Xiao-Dong Su	1017
25-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-072: Solving the phase problem without experimental phasing			CHAIR	0	Leonard Chavas	752
25-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-072: Solving the phase problem without experimental phasing	290	Structure determination and annotation of serendipitously crystallized proteins	Oral 30 mins	1	Prof Mathur R Murthy	682
25-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-072: Solving the phase problem without experimental phasing	1119	De novo in-vivo protein crystal structure: is experimental phasing required?	Oral 30 mins	2	Dr Pierre Montaville	1439
25-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-072: Solving the phase problem without experimental phasing	1428	Solving structures from in cellulose crystallized proteins: strategies and bottlenecks	Oral 30 mins	3	Prof Lars Redecke	645
25-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-072: Solving the phase problem without experimental phasing	1098	ContaMiner and ContaBase: Automated identification of unwantedly crystallized protein contaminants	Oral 30 mins	4	Prof Stefan T Arold	1426
25-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-072: Solving the phase problem without experimental phasing	220	New in the ARCIMBOLDO toolbox for phasing with small fragments	Oral 15 mins	5	Ms Claudia Lucía Millán Nebot	406
25-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-072: Solving the phase problem without experimental phasing	1439	Unconventional Molecular Replacement for Helical Transmembrane Proteins using AMPLE	Oral 15 mins	6	Mr Felix Simkovic	1657
26-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-073: Minimizing radiation damage			CHAIR	0	Mike Hough	631
26-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-073: Minimizing radiation damage	561	Radiation Damage in Macromolecular Crystallography: the current knowns and unknowns	Oral 30 mins	1	Prof Elspeth F. Garman	850
26-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-073: Minimizing radiation damage	1646	Radiation damage in electron cryomicroscopy (cryoEM)	Oral 30 mins	2	Dr Richard Henderson	77
26-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-073: Minimizing radiation damage	849	Radiation Damage in Protein Crystallography at X-ray Free-electron Lasers	Oral 30 mins	3	Dr Karol Jan Nass	1214
26-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-073: Minimizing radiation damage	788	Study and mitigation of radiation damage on the P12BioSAXS beamline	Oral 30 mins	4	Dr Clement Emmanuel Blanchet	1182

Date	Time	Hall	Theme	Microsymposium (MS)	ABS-Num.	Abstract Title	Presentation Type	Sequence	Chair/Author Name	Database ID
26-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-073: Minimizing radiation damage	1775	Low-dose X-ray structure analysis of cytochrome oxidase utilizing high-energy X-rays	Oral 15 mins	5	Dr Go Ueno	1875
26-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-073: Minimizing radiation damage	920	Cryoprotection without cryoprotectant	Oral 15 mins	6	Dr Yvonne Thielmann	1286

Date	Time	Hall	Theme	Microsymposium (MS)	ABS-Num.	Abstract Title	Presentation Type	Sequence	Chair/Author Name	Database ID
26-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-074: Porous framework materials for catalysis and renewable energy			CHAIR	0	Christian Doonan	1799
26-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-074: Porous framework materials for catalysis and renewable energy	1964	Porous crystals from the vapor phase: MOF-CVD	Oral 30 mins	1	Prof Rob Ameloot	2116
26-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-074: Porous framework materials for catalysis and renewable energy	1670	MOF Bio-composites for Biocatalysis	Oral 30 mins	2	Prof Paolo Falcaro	1822
26-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-074: Porous framework materials for catalysis and renewable energy	2039	Structural Studies of small molecules adsorbed in MOFs	Oral 30 mins	3	Dr Craig Martin Brown	2241
26-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-074: Porous framework materials for catalysis and renewable energy	2038	Guest induced structural deformation of metal-organic polyhedra	Oral 30 mins	4	Prof Shuhei Furukawa	2239
26-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-074: Porous framework materials for catalysis and renewable energy	157	Coordination Polymer Glass for Bio-inspired Photoelectric Conversion Application	Oral 15 mins	5	Dr Sanjog S. Nagarkar	466
26-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-074: Porous framework materials for catalysis and renewable energy	153	Tandem Catalysis by in-situ Generated Microporous COF-Pd Nanoparticle Hybrids	Oral 15 mins	6	Mr Mohitosh Bhadra	229
26-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-075: Tailored properties of molecular co-crystals			CHAIR	0	Srinivasulu Aitipamula	879
26-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-075: Tailored properties of molecular co-crystals			CHAIR	0	Susan Bourne	973
26-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-075: Tailored properties of molecular co-crystals	986	Regulatory classification of cocrystals and its implications on drug development	Oral 30 mins	1	Dr Sreenivas Lingireddy	1331
26-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-075: Tailored properties of molecular co-crystals	899	Multi-component crystals as selective hosts	Oral 30 mins	2	Prof Delia Ann Haynes	916

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26-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-075: Tailored properties of molecular co-crystals	1181	Optimizing co-crystal screens using a data-driven machine learning method	Oral 30 mins	3	Prof Richard Ian Cooper	1498
26-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-075: Tailored properties of molecular co-crystals	1895	Exploring cocrystallization of Curcumin	Oral 15 mins	4	Ms Jenna Marie Skieneh	2047
26-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-075: Tailored properties of molecular co-crystals	1712	Crystal engineering solutions to improve pharmacokinetic properties of nutraceuticals	Oral 15 mins	5	Dr Anil Kumar Kruthiventi	1853
26-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-075: Tailored properties of molecular co-crystals	854	Co-crystallisation and phase-transition: from Pharmaceuticals to thermochromics	Oral 15 mins	6	Dr Anuradha Pallipurath Radhakrishnan	1237
26-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-075: Tailored properties of molecular co-crystals	101	Crystal engineering of zwitterionic drug to neutral cocrystals	Oral 15 mins	7	Mr Anilkumar Gunnam	161
26-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-076: Diffuse scattering in crystalline structures			CHAIR	0	Ray Withers	318
26-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-076: Diffuse scattering in crystalline structures			CHAIR	0	Bernardo Barbiellini	2080
26-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-076: Diffuse scattering in crystalline structures	1245	Strongly Correlated Disorder and the Procrystalline State	Oral 30 mins	1	Prof Andrew Goodwin	1534
26-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-076: Diffuse scattering in crystalline structures	1081	Space and time correlations of polar fluctuations in dielectric materials	Oral 30 mins	2	Dr Marek Pasciak	1409
26-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-076: Diffuse scattering in crystalline structures	1266	PbTe studied by 3D- $\Delta$ PDF analysis and ab-initio simulations	Oral 30 mins	3	Dr Thomas Weber	1524
26-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-076: Diffuse scattering in crystalline structures	1576	Single crystal diffuse scattering—a solution to the phase problem?	Oral 30 mins	4	Dr Arkadiy Simonov	1726
26-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-076: Diffuse scattering in crystalline structures	605	Disordered structures in lead-free piezoelectrics	Oral 15 mins	5	Mr Patrick Kin Man Tung	1028
26-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-076: Diffuse scattering in crystalline structures	945	Diffuse single crystal scattering corrected for molecular formfactor effects	Oral 15 mins	6	Ms Ella Mara Schmidt	1299

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26-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-077: Coherence, spectroscopy and time resolved crystallography with new sources			CHAIR	0	Jan Kern	1743
26-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-077: Coherence, spectroscopy and time resolved crystallography with new sources	1001	Ultrafast Time-resolved X-ray Spectroscopies at SACLA	Oral 30 mins	1	Dr Tetsuo Katayama	1341
26-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-077: Coherence, spectroscopy and time resolved crystallography with new sources	1721	Time-resolved Serial Crystallography of Bacteriorhodopsin using Synchrotrons and X-ray Lasers	Oral 30 mins	2	Dr Joerg Standfuss	1815
26-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-077: Coherence, spectroscopy and time resolved crystallography with new sources	208	Time-resolved X-ray diffraction on Density-Waves systems	Oral 30 mins	3	Dr Sylvain Ravy	554
26-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-077: Coherence, spectroscopy and time resolved crystallography with new sources	1906	Time-resolved study of molecular crystals, with anomalously short Br...Br contacts	Oral 30 mins	4	Dr Krishnayan Basuroy	2010
26-08-2017	1030-1305	MR 1.05	Instrumentation techniques and/or Computation	MS-077: Coherence, spectroscopy and time resolved crystallography with new sources	1325	Coherent X-Ray Experiments at 9000 Hz	Oral 30 mins	5	Dr Stefan Brandstetter	1585
26-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-078: Advances in high-pressure crystallographic methods			CHAIR	0	Prof. Goutam Dev Mukherjee	1804
26-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-078: Advances in high-pressure crystallographic methods			CHAIR	0	Kamil Dziubek	1549
26-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-078: Advances in high-pressure crystallographic methods	123	Melting dynamics of ices by time-resolved light scattering	Oral 30 mins	1	Margherita Citroni	413
26-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-078: Advances in high-pressure crystallographic methods	1720	Novel platform for high-pressure static and dynamic X-ray diffraction experiments	Oral 30 mins	2	Dr Karen Appel	1599
26-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-078: Advances in high-pressure crystallographic methods	887	Towards joint high-pressure X-ray and neutron single-crystal diffraction	Oral 30 mins	3	Prof Garry James McIntyre	1263
26-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-078: Advances in high-pressure crystallographic methods	1170	Single-crystal neutron diffraction in diamond anvil cells with hot neutrons	Oral 30 mins	4	Dr Andrzej Grzechnik	1405



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26-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-078: Advances in high-pressure crystallographic methods	1247	Phase transitions of VO2 above 200GPa: XRD and first-principles calculations	Oral 15 mins	5	Dr Arthur Haozhe Liu	1541
26-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-078: Advances in high-pressure crystallographic methods	1350	When one crystal is not enough	Oral 15 mins	6	Dr Eric Hovestreydt	1601
26-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-079: Topological insulators			CHAIR	0	Dharmalingam Prabhakaran	293
26-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-079: Topological insulators			CHAIR	0	Devashibhai Thakarshibhai Adroja	703
26-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-079: Topological insulators	473	Neutron scattering study of the Kondo insulators CeT2Al10 (T=Fe,Ru,Os)	Oral 30 mins	1	Dr Devashibhai Thakarshibhai Adroja	703
26-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-079: Topological insulators	501	Topological behaviour of Ternary non-symmorphic crystals KZnX (X=P,As,Sb)	Oral 30 mins	2	Dr Atahar Parveen	751
26-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-079: Topological insulators	2104	Crystal growth of Topological insulators	Oral 30 mins	3	Dr Dharmalingam Prabhakaran	293
26-08-2017	1030-1305	MR 2.02	Special Activities	MS-080: Emerging science in the emerging world			CHAIR	0	Claude Lecomte	667
26-08-2017	1030-1305	MR 2.02	Special Activities	MS-080: Emerging science in the emerging world			CHAIR	0	Michele Zema	1493
26-08-2017	1030-1305	MR 2.02	Special Activities	MS-080: Emerging science in the emerging world	1491	SESAME Light Source: Why in the Middle East?	Oral 30 Mins	1	Dr Gihan Salah Kamel	1589
26-08-2017	1030-1305	MR 2.02	Special Activities	MS-080: Emerging science in the emerging world	282	Crystallography - As an Emerging Science. Has Ghana a place?	Oral 10 mins	2	Prof Robert Kingsford-Adaboh	562
26-08-2017	1030-1305	MR 2.02	Special Activities	MS-080: Emerging science in the emerging world	1456	NITUB - a scientific emerging network.	Oral 10 mins	3	Prof Altaf Hussain	359
26-08-2017	1030-1305	MR 2.02	Special Activities	MS-080: Emerging science in the emerging world	1564	Crystallography in the developing world: Experiences in Africa and beyond	Oral 10 mins	4	Ms Suzanna Clare Ward	178
26-08-2017	1030-1305	MR 2.02	Special Activities	MS-080: Emerging science in the emerging world	1638	Brazilian Synchrotron Light Laboratory. History and scientific challenges for crystallographers	Oral 10 mins	5	Prof Aldo Felix Craievich	1002

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26-08-2017	1030-1305	MR 2.02	Special Activities	MS-080: Emerging science in the emerging world	1945	The Indo-Italian cooperation at the Elettra Synchrotron Radiation Facility	Oral 10 mins	6	Dr Andrea Lausi	2088
26-08-2017	1030-1305	MR 2.02	Special Activities	MS-080: Emerging science in the emerging world	715	Crystal growth competition, a key for crystallography emergence in Benin	Oral 10 mins	7	Ms Marielle Yasmine Agbahoungbata	727
26-08-2017	1030-1305	MR 2.02	Special Activities	MS-080: Emerging science in the emerging world	1936	Lightsources for Africa, the Americas and Middle East Project (LAAMP)	Oral 10 mins	8	Prof Sandro Scandolo	1583
26-08-2017	1030-1305	MR 2.02	Special Activities	MS-080: Emerging science in the emerging world	225	Graphene based inkjet-printable electrodes for Dye sensitized solar cells	Oral 10 mins	9	Dr David Dodoo-Arhin	535
26-08-2017	1030-1305	MR 2.02	Special Activities	MS-080: Emerging science in the emerging world	649	Novel Porous Supramolecular Networks : Synthesis, characterization and Sorption Properties	Oral 10 mins	10	Dr Patrice Kenfack Tsobnang	821
26-08-2017	1030-1305	MR 2.02	Special Activities	MS-080: Emerging science in the emerging world	1702	X-ray structure characterization of metal-benzoic acid organic complexes	Oral 10 mins	11	Mr Rishad Kunafiev	981
26-08-2017	1030-1305	MR 2.02	Special Activities	MS-080: Emerging science in the emerging world	1953	Study of properties of Cambodian clays by X-ray diffraction technique	Oral 10 mins	12	Dr Kim Ngun Bun	2104
26-08-2017	1030-1305	MR 2.02	Special Activities	MS-080: Emerging science in the emerging world	1412	Chemical speciation of drinking water in Nuwaragampalatha.	Oral 5 Mins	13	Ms Dinesha Hansamali Perera	1637
26-08-2017	1030-1305	MR 2.02	Special Activities	MS-080: Emerging science in the emerging world	997	How to boost the teaching of crystallography in emerging countries?	Oral 10 mins	14	Prof Tonle Kenfack Ignas	435
26-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-081: Macromolecular machinery			CHAIR	0	Richard Charles Garratt	1039
26-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-081: Macromolecular machinery			CHAIR	0	Soichi Wakatsuki	814
26-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-081: Macromolecular machinery	1363	Structure based analysis of the Type III Secretion Injectisome	Oral 30 mins	1	Prof Catherine Natalie Strynadka	1605
26-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-081: Macromolecular machinery	1719	Structural basis for processive transcription antitermination	Oral 30 mins	2	Prof Markus C. Wahl	1860
26-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-081: Macromolecular machinery	1026	Ezrin, monomeric and dimeric, characterised by crystallography and SAXS	Oral 30 mins	3	Dr Anthony Patrick Duff	1359

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26-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-081: Macromolecular machinery	955	COMMANDER COMPLEX: a new endosomal protein sorting platform	Oral 30 mins	4	Dr Rajesh Ghai	1314
26-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-081: Macromolecular machinery	223	Two-Component Systems in Bacteria: how is the signal unidirectionally transmitted?	Oral 15 mins	5	Mr Juan Andres Imelio	560
26-08-2017	1030-1305	MR 2.03-2.04	Biological Macromolecules (Function)	MS-081: Macromolecular machinery	1743	Unraveling the structural dynamics of the Type II secretion system.	Oral 15 mins	6	Dr Mangayarkarasi Nivaskumar	741
26-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-082: Techniques and insights into macromolecular crystallization			CHAIR	0	Anna Schenk	2018
26-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-082: Techniques and insights into macromolecular crystallization			CHAIR	0	Abel Moreno	1831
26-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-082: Techniques and insights into macromolecular crystallization	1693	Crystal growth of inorganic, organic, and biological macromolecules in gels	Oral 30 mins	1	Dr Maria J. Rosales-Hoz	1841
26-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-082: Techniques and insights into macromolecular crystallization	453	Enhancing the success of crystallization: strategies and techniques	Oral 30 mins	2	Dr Lata Govada	851
26-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-082: Techniques and insights into macromolecular crystallization	176	Overcoming two major chokepoints of protein crystallography with lanthanide complexes.	Oral 30 mins	3	Dr François Riobé	331
26-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-082: Techniques and insights into macromolecular crystallization	652	A new crystallization plate for efficient protein crystallization	Oral 30 mins	4	Prof Da-Chuan Yin	1071
26-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-082: Techniques and insights into macromolecular crystallization	456	Microseed matrix-screening for crystallization: theory, practice and a new technique	Oral 15 mins	5	Mr Patrick Douglas Shaw Stewart	853
26-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-082: Techniques and insights into macromolecular crystallization	451	Design and application of crystallization aids comprising DARPIn domains.	Oral 15 mins	6	Dr Peer Mittl	179

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26-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-083: Polyoxometalates as building blocks for functional materials			CHAIR	0	Arunachalam Ramanan	102
26-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-083: Polyoxometalates as building blocks for functional materials			CHAIR	0	Soumyajit Roy	1512
26-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-083: Polyoxometalates as building blocks for functional materials	1597	Ligand-induced Self-Assembly of Polyoxometalates	Oral 30 mins	1	Prof Bernold Hasenknopf	1750
26-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-083: Polyoxometalates as building blocks for functional materials	1625	Polyoxometalate Based Metal-organic Framework	Oral 30 mins	2	Prof Chunying Duan	1603
26-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-083: Polyoxometalates as building blocks for functional materials	541	Electronically wired polyoxometalate-based networks in the crystalline states	Oral 30 mins	3	Dr Ryo Tsunashima	960
26-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-083: Polyoxometalates as building blocks for functional materials	65	Supramolecular Chemistry of Polyoxometalates: from Small Clusters to Giant Keplerates	Oral 30 mins	4	Prof Samar Das	247
26-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-083: Polyoxometalates as building blocks for functional materials	1980	Hybrid polyoxometalates as multifunctional materials, photoresists, green catalyst and antioxidants	Oral 15 mins	5	Dr Pradeep Chullikkattil Parameswaran	2146
26-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-083: Polyoxometalates as building blocks for functional materials	829	EXPLORATION OF SOFT OXOMETALATES IN PATTERNING AND ALLIED STUDIES	Oral 15 mins	6	Ms Preethi Thomas	1213
26-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-084: Soft organic and inorganic materials: Gelation and crystallization			CHAIR	0	Cheng-Yong Su	958
26-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-084: Soft organic and inorganic materials: Gelation and crystallization			CHAIR	0	Parthasarathi Dastidar	519
26-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-084: Soft organic and inorganic materials: Gelation and crystallization	1293	Phenylalanine gelation and its dynamics studied through crystal structure analysis.	Oral 30 mins	1	Dr Gareth Owen Lloyd	1566

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26-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-084: Soft organic and inorganic materials: Gelation and crystallization	260	Pincer Molecular Metallogels: A New Platform for Visual Recognition	Oral 30 mins	2	Prof Tao Tu	541
26-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-084: Soft organic and inorganic materials: Gelation and crystallization	1225	Fluorescent Vesicles Based on Aggregation Induced Emission Compound	Oral 30 mins	3	Prof Yun Yan	1466
26-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-084: Soft organic and inorganic materials: Gelation and crystallization	170	An Easy Access to Supramolecular Gels of Tolfenamic Acid	Oral 30 mins	4	Ms Rumana Parveen	480
26-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-084: Soft organic and inorganic materials: Gelation and crystallization	312	Low-molecular-weight amino-acid-based derivatives: from organogels to single crystals and mesocrystals	Oral 15 mins	5	Dr Florencia Di Salvo	561
26-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-084: Soft organic and inorganic materials: Gelation and crystallization	867	Fluorescent Zwitterionic Spirocyclic Meisenheimer Complex: X-Ray Structure and Function	Oral 15 mins	6	Mr Tanmay Das	1243
26-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-085: Dynamic phenomena and material functionality from inelastic x-ray scattering			CHAIR	0	Yoshiharu Sakurai	804
26-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-085: Dynamic phenomena and material functionality from inelastic x-ray scattering			CHAIR	0	Eiji Nishibori	1315
26-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-085: Dynamic phenomena and material functionality from inelastic x-ray scattering	1972	Inelastic X-Ray Scattering as a Unique Probe of Complex Materials	Oral 30 mins	1	Prof Arun Bansil	2130
26-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-085: Dynamic phenomena and material functionality from inelastic x-ray scattering	1317	Iron(III, IV, V)-oxo complexes studied by nuclear resonance vibrational spectroscopy	Oral 30 mins	2	Dr Yisong Guo	1582
26-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-085: Dynamic phenomena and material functionality from inelastic x-ray scattering	396	Magnetization switching behavior for CoFeB/MgO and CoFeB/Ta multilayer films	Oral 30 mins	3	Prof Hiroshi Sakurai	804
26-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-085: Dynamic phenomena and material functionality from inelastic x-ray scattering	1622	Determination of proton conduction in olivine and hydrogarnet	Oral 30 mins	4	Mr Sarath Patabendi Gedara	1770

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26-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-085: Dynamic phenomena and material functionality from inelastic x-ray scattering	48	Electronic Structure of Oxide Electrode Materials studied by Compton Profiles	Oral 30 mins	5	Dr Kosuke Suzuki	147
26-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-086: Accurate high resolution diffraction studies at high pressure			CHAIR	0	Krzysztof Wozniak	787
26-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-086: Accurate high resolution diffraction studies at high pressure			CHAIR	0	Nicola Casati	2075
26-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-086: Accurate high resolution diffraction studies at high pressure	373	Novel nitrogen-rich iron nitrides synthesized at high-pressure high-temperature conditions	Oral 30 mins	1	Dr Maxim Bykov	788
26-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-086: Accurate high resolution diffraction studies at high pressure	1187	Accurate structures of diamond under high- pressure and temperature.	Oral 30 mins	2	Ms Yuuka Deguchi	1354
26-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-086: Accurate high resolution diffraction studies at high pressure	1395	High-pressure studies for understanding mechanical effects on chemical reactions	Oral 30 mins	3	Dr Boris Zakharov	1385
26-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-086: Accurate high resolution diffraction studies at high pressure	1684	In-situ stability of carbonates in presence of mantle phases	Oral 30 mins	4	Dr Karen Appel	1599
26-08-2017	1455-1730	MR 1.05	Instrumentation techniques and/or Computation	MS-086: Accurate high resolution diffraction studies at high pressure	1944	THE HIGH PRESSURE DIFFRACTION BEAMLINe "XPRESS" AT ELETTRA	Oral 30 mins	5	Dr Andrea Lausi	2088
26-08-2017	1455-1730	MR 1.06	Special Activities	MS-087: How does crystallography help you in your career?			CHAIR	0	Ashwini Nangia	297
26-08-2017	1455-1730	MR 1.06	Special Activities	MS-087: How does crystallography help you in your career?			CHAIR	0	Soorya N	991
26-08-2017	1455-1730	MR 1.06	Special Activities	MS-087: How does crystallography help you in your career?	1995	Important Role of Crystallography in Pharmaceutical Development	Oral 30 mins	1	Dr Sudhir Nambiar	2172
26-08-2017	1455-1730	MR 1.06	Special Activities	MS-087: How does crystallography help you in your career?	1856	Crystal Engineering for Career Opportunities in Pharmaceutical Research Innovation	Oral 30 mins	2	Prof Anant Paradkar	1976
26-08-2017	1455-1730	MR 1.06	Special Activities	MS-087: How does crystallography help you in your career?	647	A view from a Latin American Crystallography Laboratory	Oral 30 mins	3	Prof José Miguel Delgado	989
26-08-2017	1455-1730	MR 1.06	Special Activities	MS-087: How does crystallography help you in your career?	2062	Crystallography in the globes largest chemical company	Oral 30 mins	4	Dr Martin Viertelhaus	2315

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26-08-2017	1455-1730	MR 1.06	Special Activities	MS-087: How does crystallography help you in your career?	569	Celebrating 75 years of the Powder Diffraction File™	Oral 30 mins	5	Dr Soorya N Kabekkodu	991
26-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-088: Hybrid perovskites			CHAIR	0	Roberto Mosca	1995
26-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-088: Hybrid perovskites	1229	Hybrid Perovskite Crystals: Surface Restructuring under Humid Ambient	Oral 30 mins	1	Dr Murali Banavoth	1530
26-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-088: Hybrid perovskites	1038	Photoluminescence in lead halide perovskites and the role of defects	Oral 30 mins	2	Dr Ajay Ram Srimath Kandada	1376
26-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-088: Hybrid perovskites	415	Structure, optical studies of 2D hybrid perovskite for photovoltaic applications	Oral 30 mins	3	Dr Seham Kamal Abdel-Aal	806
26-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-088: Hybrid perovskites	1771	Local structure of lead halide perovskites for photovoltaic applications	Oral 30 mins	4	Ms Jiaxun Liu	1900
26-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-088: Hybrid perovskites	1329	Nucleation and self-assembly of CsPbX <sub>3</sub> Perovskite Nanocrystals	Oral 30 mins	5	Mr Sudipta Seth	1591
26-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-089: Chemistry and physics of modulated and composite crystals			CHAIR	0	Siegbert Schmid	1514
26-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-089: Chemistry and physics of modulated and composite crystals			CHAIR	0	Thomas Doert	437
26-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-089: Chemistry and physics of modulated and composite crystals	398	Dynamic studies of incommensurate materials	Oral 30 mins	1	Prof Sven Lidin	588
26-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-089: Chemistry and physics of modulated and composite crystals	1992	Transitions toward complex electronic states and superperiodic structures in MPTBp	Oral 30 mins	2	Dr Olivier Pérez	2171
26-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-089: Chemistry and physics of modulated and composite crystals	1371	Mullite - Towards a unified superspace model	Oral 30 mins	3	Mr Paul Benjamin Klar	54
26-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-089: Chemistry and physics of modulated and composite crystals	1418	Phase transitions and crystal structures of $\eta''$ -Cu(3+x)Si and $\eta'''$ -Cu(3+x)Si	Oral 30 mins	4	Ms Cinthia Antunes Correa	1628
26-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-089: Chemistry and physics of modulated and composite crystals	1278	Modulated and high Z' phases in $\Lambda$ -Cobalt(III) sepulchrate trinitrate	Oral 15 mins	5	Dr Somnath Dey	1519
26-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-089: Chemistry and physics of modulated and composite crystals	883	The Auln 1:1 phase and its siblings	Oral 15 mins	6	Ms Laura Folkers	1215

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26-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-090: Spectroscopy applications in biologically relevant systems			CHAIR	0	Bhoopesh Mishra	53
26-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-090: Spectroscopy applications in biologically relevant systems			CHAIR	0	Sofia Diaz-Moreno	2014
26-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-090: Spectroscopy applications in biologically relevant systems	1003	Synchrotron Spectroscopy and Imaging in Unraveling Bacterial Surface Metal Interactions	Oral 30 mins	1	Prof Satish Myneni	1343
26-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-090: Spectroscopy applications in biologically relevant systems	886	Post-translation tyrosine phosphorylation switches Cytochrome c dynamics.	Oral 30 mins	2	Prof Antonio J Diaz Quintana	374
26-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-090: Spectroscopy applications in biologically relevant systems	1890	Spectroscopy Applications in Biologically Relevant Systems	Oral 30 mins	3	Dr Ritimukta Sarangi	1996
26-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-090: Spectroscopy applications in biologically relevant systems	1445	Time-Resolved Structural Biology Benefits from Complementary Methods	Oral 30 mins	4	Dr Allen Milster Orville	1570
26-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-090: Spectroscopy applications in biologically relevant systems	581	Picosecond to Microsecond TR-XAS: Intermediates in the photolysis of MethylCobalamin	Oral 15 mins	5	Dr Ganesh Subramanian	1001
26-08-2017	1455-1730	MR 2.03-2.04	Biological Macromolecules (Function)	MS-090: Spectroscopy applications in biologically relevant systems	680	XAS structural insights into Cu binding with amyloid A $\beta$ 4-y peptides	Oral 15 mins	6	Ms Ruwini Supeshala Kumari Ekanayake	1083
27-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-091: Expression of macromolecular complexes			CHAIR	0	Areej Abuhammad	1265
27-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-091: Expression of macromolecular complexes	328	Streamlining protein complex production using multiprotein expression technologies	Oral 30 mins	1	Dr Yan Nie	496
27-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-091: Expression of macromolecular complexes	1093	Versatile medium-throughput strategies for recombinant expression screening in structural biology	Oral 30 mins	2	Dr Federico Forneris	761



Date	Time	Hall	Theme	Microsymposium (MS)	ABS-Num.	Abstract Title	Presentation Type	Sequence	Chair/Author Name	Database ID
27-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-091: Expression of macromolecular complexes	335	Expanding the Toolbox: Recent Advances in Multiprotein Expression Systems.	Oral 30 mins	3	Dr Kapil Kumar Gupta	738
27-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-091: Expression of macromolecular complexes	333	In vivo selective deuteration of complex biological systems	Oral 30 mins	4	Mr Benjamin Brocco	528
27-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-091: Expression of macromolecular complexes	1062	The GM-CSF Receptor - Mechanisms for Affinity Conversion and Signalling	Oral 15 mins	5	Dr Sophie Elizabeth Broughton	1394
27-08-2017	1030-1305	Hall 4	Biological Macromolecules (Structure)	MS-091: Expression of macromolecular complexes	1161	Structure of 3-nitrotoluene dioxygenase from diaphorobacter sp. strain DS2	Oral 15 mins	6	Prof Gurunath Ramanathan	1467

Date	Time	Hall	Theme	Microsymposium (MS)	ABS-Num.	Abstract Title	Presentation Type	Sequence	Chair/Author Name	Database ID
27-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-092: Bio-compatible porous materials for drug delivery			CHAIR	0	Paolo Falcaro	1822
27-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-092: Bio-compatible porous materials for drug delivery			CHAIR	0	Alessia Bacchi	1194
27-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-092: Bio-compatible porous materials for drug delivery	749	Chitosan-engineered Metal-Organic Frameworks as oral drug nanocarriers	Oral 30 mins	1	Dr Patricia Horcajada	1144
27-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-092: Bio-compatible porous materials for drug delivery	119	The chemistry of $\delta$ metal-organic framework nanoparticles	Oral 30 mins	2	Dr Stefan Wuttke	399
27-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-092: Bio-compatible porous materials for drug delivery	408	ENCAPSULATION OF DIPHTHERIA ANATOXIN INTO ORDERED MESOPOROUS SILICA	Oral 30 mins	3	Prof Marcia Carvalho De Abreu Fantini	234
27-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-092: Bio-compatible porous materials for drug delivery	1468	Structural model of Cowlesite by fast electron diffraction tomography	Oral 30 mins	4	Dr Mauro Gemmi	1673
27-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-092: Bio-compatible porous materials for drug delivery	864	Biodegradable containers based on nanostructured polycrystals obtained by controlled crystallization	Oral 15 mins	5	Ms Daria Trushina	1247
27-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-092: Bio-compatible porous materials for drug delivery	168	Multifunctional Single-layered Vesicles Derived from Cu(II)-Metal-Organic-Polyhedra	Oral 15 mins	6	Mr Koushik Sarkar	490
27-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-093: Halogen bonding in crystal engineering			CHAIR	0	Kari Rissanen	89
27-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-093: Halogen bonding in crystal engineering			CHAIR	0	Pierangelo Metrangolo	1044
27-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-093: Halogen bonding in crystal engineering	436	Trifluoromethyl groups as halogen bond donors: the effect of group-polarizability	Oral 30 mins	1	Prof Catharine Esterhuysen	841
27-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-093: Halogen bonding in crystal engineering	1562	Directed Reactivity in Halogen-Bonded Cocrystals	Oral 30 mins	2	Prof Leonard Richard MacGillivray	1690

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27-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-093: Halogen bonding in crystal engineering	66	Crystal Engineering pi-ways for Enhanced Charge Transport	Oral 30 mins	3	Dr Mahesh Hariharan	253
27-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-093: Halogen bonding in crystal engineering	318	"Organic fluorine" in stabilizing crystal structures: Does it matter?	Oral 30 mins	4	Dr Angshuman Roychoudhury	716
27-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-093: Halogen bonding in crystal engineering	776	Ion pair interactions in noble metal complexes with halogen atoms	Oral 30 mins	5	Prof Luciano Marchio'	914
27-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-094: Phase-plates : Improving resolution in CryoEM			CHAIR	0	Radostin Danev	1430
27-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-094: Phase-plates : Improving resolution in CryoEM			CHAIR	0	Bart Buijsse	2070
27-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-094: Phase-plates : Improving resolution in CryoEM	709	3.9Å phase plate cryo-EM reconstruction of the nucleosome core particle	Oral 30 mins	1	Dr Eugene Yue Dao Chua	1117
27-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-094: Phase-plates : Improving resolution in CryoEM	1142	GPCR activation: An intertwined history of crystallography and EM	Oral 30 mins	2	Dr Mazdak Radjainia	1448
27-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-094: Phase-plates : Improving resolution in CryoEM	1963	Spotiton: A new method for vitrifying samples for cryoEM	Oral 30 mins	3	Dr Venkata Prasad Dandey	2108
27-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-094: Phase-plates : Improving resolution in CryoEM	1815	The structure of the cyanide dihydratase (CynD) from Bacillus pumilus	Oral 30 mins	4	Prof Bryan Trevor Sewell	1502
27-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-094: Phase-plates : Improving resolution in CryoEM	1432	Single Particle Cryo-EM of Macromolecular Complexes at Near-atomic Resolution.	Oral 30 mins	5	Mr Eugene B. Pichkur	1643
27-08-2017	1030-1305	MR 1.05	Special Activities	MS-095: Crystallography for Space Sciences			CHAIR	0	Hanna Dabkowska	604
27-08-2017	1030-1305	MR 1.05	Special Activities	MS-095: Crystallography for Space Sciences			CHAIR	0	Juan Manuel Garcia Ruiz	2042
27-08-2017	1030-1305	MR 1.05	Special Activities	MS-095: Crystallography for Space Sciences	578	Mineralogical Results from the Mars Science Laboratory Rover Curiosity	Oral 30 mins	1	Dr David Frederick Blake	999
27-08-2017	1030-1305	MR 1.05	Special Activities	MS-095: Crystallography for Space Sciences	1433	Mineralogy and crystallography of return samples from primitive asteroids	Oral 30 mins	2	Prof Tomoki Nakamura	1655

Date	Time	Hall	Theme	Microsymposium (MS)	ABS-Num.	Abstract Title	Presentation Type	Sequence	Chair/Author Name	Database ID
27-08-2017	1030-1305	MR 1.05	Special Activities	MS-095: Crystallography for Space Sciences	229	Prospects for organic minerals on Saturn's moon Titan	Oral 15 mins	3	Dr Helen Elizabeth Maynard-Casely	514
27-08-2017	1030-1305	MR 1.05	Special Activities	MS-095: Crystallography for Space Sciences	1287	Early stages of grain formation studied by microgravity experiments	Oral 15 mins	4	Prof Yuki Kimura	1446
27-08-2017	1030-1305	MR 1.05	Special Activities	MS-095: Crystallography for Space Sciences	530	Ordering phenomena in minerals: the Verwey phase of natural magnetite	Oral 15 mins	5	Ms Giuditta Perversi	924
27-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-096: XAFS of materials for clean energy			CHAIR	0	Steve M. Heald	937
27-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-096: XAFS of materials for clean energy	574	-ray Absorption Spectroscopy Applied to Solar Absorbers	Oral 30 mins	1	Prof Michael F Toney	996
27-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-096: XAFS of materials for clean energy	334	A SPring-8 New Beam Line for the Fuel Cell Analysis	Oral 30 mins	2	Prof Kiyotaka Asakura	736
27-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-096: XAFS of materials for clean energy	1753	Operando XAS studies on catalysts for energy related processes	Oral 30 mins	3	Dr Henning Lichtenberg	1303
27-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-096: XAFS of materials for clean energy	331	Element specific channels in photo-excitation of V-doped TiO2 nanoparticles	Oral 30 mins	4	Mr Giacomo Rossi	439
27-08-2017	1030-1305	MR 1.06	Instrumentation techniques and/or Computation	MS-096: XAFS of materials for clean energy	1104	Changes in local electronic structure on the Si/TiO2/Fe2O3 photo-catalysts	Oral 30 mins	5	Mr Anurag Kawde	1435
27-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-097: Functional magnetic materials			CHAIR	0	Jose-Antonio Alonso	591
27-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-097: Functional magnetic materials			CHAIR	0	Daniel Shoemaker	1823
27-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-097: Functional magnetic materials	499	Using polyhedral distortions to understand structure-property behaviour.	Oral 30 mins	1	Dr James Cumby	909
27-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-097: Functional magnetic materials	167	Heavy Metal: Magneto-Structural Relationships in Ir and Os Oxides.	Oral 30 mins	2	Prof Brendan James Kennedy	489
27-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-097: Functional magnetic materials	1502	Magnetic, magnetostructural and magnetoelectric properties of cobalt-based oxides	Oral 30 mins	3	Prof Jose Luis Garcia-Muñoz	1506
27-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-097: Functional magnetic materials	547	Unusual magnetic ordered metallic state in EuNiO3 under pressure	Oral 30 mins	4	Prof Hisao Kobayashi	962

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27-08-2017	1030-1305	MR 2.01	Materials and Minerals	MS-097: Functional magnetic materials	1736	Swinging Symmetry, Structural Phase Transitions and Physical Properties of RETGa3	Oral 30 mins	5	Prof Sebastian Chirambatte Peter	1877
27-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-098: Recent advances in quasicrystal research			CHAIR	0	Katariina Pussi	728
27-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-098: Recent advances in quasicrystal research			CHAIR	0	Yasushi Ishii	2071
27-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-098: Recent advances in quasicrystal research	424	Canonical-cell approach to icosahedral quasicrystals and their approximants	Oral 30 mins	1	Dr Nobuhisa Fujita	831
27-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-098: Recent advances in quasicrystal research	1357	Lattice dynamics of the complex metallic alloys o-Al13Co4	Oral 30 mins	2	Dr Marc De Boissieu	1608
27-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-098: Recent advances in quasicrystal research	534	Simple particles, complex structures	Oral 30 mins	3	Dr Julia Dshemuchadse	945
27-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-098: Recent advances in quasicrystal research	509	Templated Quasicrystalline Thin Film of Molecules: Recent Extended Study	Oral 30 mins	4	Dr Hem Raj Sharma	920
27-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-098: Recent advances in quasicrystal research	1709	Atomic structures of the Sc-Zn and R-Cd icosahedral quasicrystals	Oral 15 mins	5	Dr Tsunetomo Yamada	1849
27-08-2017	1030-1305	MR 2.02	Physical and/or Fundamental	MS-098: Recent advances in quasicrystal research	1920	$\gamma$ -brass related complex phases in Rh-Cd binary system	Oral 15 mins	6	Dr Partha Pratim Jana	2024

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27-08-2017	1030-1305	MR 2.03-2.04	Special Activities	MS-099: Crystallographic data and structure validation from data collection to publication - IUCr setting standards			CHAIR	0	Wladek Minor	1844
27-08-2017	1030-1305	MR 2.03-2.04	Special Activities	MS-099: Crystallographic data and structure validation from data collection to publication - IUCr setting standards			CHAIR	0	Anthony Linden	96
27-08-2017	1030-1305	MR 2.03-2.04	Special Activities	MS-099: Crystallographic data and structure validation from data collection to publication - IUCr setting standards	469	What makes a structure report valid?	Oral 30 mins	1	Prof Anthony Louis Spek	100
27-08-2017	1030-1305	MR 2.03-2.04	Special Activities	MS-099: Crystallographic data and structure validation from data collection to publication - IUCr setting standards	496	Towards Archiving Raw Diffraction Images for Validating Crystal Structures.	Oral 30 mins	2	Dr Loes M.J. Kroon-Batenburg	398
27-08-2017	1030-1305	MR 2.03-2.04	Special Activities	MS-099: Crystallographic data and structure validation from data collection to publication - IUCr setting standards	285	Frauds in small molecule crystallography	Oral 30 mins	3	Prof James Simpson	677
27-08-2017	1030-1305	MR 2.03-2.04	Special Activities	MS-099: Crystallographic data and structure validation from data collection to publication - IUCr setting standards	154	DFT-D and the validation of crystal structures from XRPD	Oral 30 mins	4	Dr Cornelis Jan Van De Streek	460
27-08-2017	1030-1305	MR 2.03-2.04	Special Activities	MS-099: Crystallographic data and structure validation from data collection to publication - IUCr setting standards	949	wwPDB OneDep Validation Services	Oral 30 mins	5	Dr John Westbrook	805

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27-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-100: Structure determination of biological macromolecule complexes by Cryo-EM			CHAIR	0	Edward N. Baker	303
27-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-100: Structure determination of biological macromolecule complexes by Cryo-EM			CHAIR	0	Yifan Cheng	2152
27-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-100: Structure determination of biological macromolecule complexes by Cryo-EM	359	CryoEM Structure of Dynamin-like MxB in Assembly	Oral 30 mins	1	Prof Peijun Zhang	771
27-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-100: Structure determination of biological macromolecule complexes by Cryo-EM	319	Revealing the atomic-level organization of a bacterial microinjection nanodevice	Oral 30 mins	2	Prof Alok K. Mitra	717
27-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-100: Structure determination of biological macromolecule complexes by Cryo-EM	1955	Structural basis of protein translocation by the Vps4-Vta1 AAA ATPase	Oral 30 mins	3	Dr Christopher Hill	2107
27-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-100: Structure determination of biological macromolecule complexes by Cryo-EM	128	Model-building using cryo-EM and crystallographic maps	Oral 30 mins	4	Dr Thomas Terwilliger	109
27-08-2017	1455-1730	Hall 4	Biological Macromolecules (Structure)	MS-100: Structure determination of biological macromolecule complexes by Cryo-EM	1155	Structure of Elongation Factor 4 Bound to the Ribosome	Oral 30 mins	5	Dr Veerendra Kumar	159
27-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-101: Porous framework materials for sensing			CHAIR	0	Stuart Batten	1855
27-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-101: Porous framework materials for sensing			CHAIR	0	Hai-Long Jiang	498
27-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-101: Porous framework materials for sensing	249	Metal-organic Frameworks (MOFs) for Sensing Applications	Oral 30 mins	1	Dr Sujit K. Ghosh	618

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27-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-101: Porous framework materials for sensing	404	Understanding selective Cu <sup>2+</sup> detection by Ln <sup>3+</sup> complexes through crystallography	Oral 30 mins	2	Mr Soumyabrata Roy	807
27-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-101: Porous framework materials for sensing	2006	Unique Porous Frameworks as Luminescent Probes	Oral 30 mins	3	Prof Bin Zhao	2190
27-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-101: Porous framework materials for sensing	859	Porous gel materials assembled from small molecules	Oral 30 mins	4	Dr Jianyong Zhang	958
27-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-101: Porous framework materials for sensing	51	MULTIFUNCTIONAL MATERIALS FOR SENSING OF METAL IONS AND SMALL MOLECULES	Oral 15 mins	5	Prof Sanjay K Mandal	173
27-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-101: Porous framework materials for sensing	1023	Water-Stable MOF for Recognition and Sequestration of Oxoanion Pollutants	Oral 15 mins	6	Mr Aamod Vikas Desai	558
27-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-102: Halogen bonding at the interface between small molecules and macromolecules			CHAIR	0	José A. Gavira	694
27-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-102: Halogen bonding at the interface between small molecules and macromolecules			CHAIR	0	Kana Sureshan	980
27-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-102: Halogen bonding at the interface between small molecules and macromolecules	626	Halogenation as a new tool to control peptide self-assembly	Oral 30 mins	1	Prof Pierangelo Metrangolo	1044
27-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-102: Halogen bonding at the interface between small molecules and macromolecules	1167	Halogen Bond Driven Encapsulation of Tetrahalomethanes within a Supramolecular Host	Oral 30 mins	2	Dr Anssi Peuronen	1478
27-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-102: Halogen bonding at the interface between small molecules and macromolecules	1061	Halogenated Anthrapyrazolone derivatives regulate JNK signals in inflammation	Oral 30 mins	3	Prof Tayur Guru Row	494



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27-08-2017	1455-1730	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-102: Halogen bonding at the interface between small molecules and macromolecules	596	Halogen Bonded Capsules	Oral 30 mins	4	Prof Kari Rissanen	89
27-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-103: Methods for characterizing commensurate and incommensurate magnetic structures			CHAIR	0	Margarida S. Henriques	2007
27-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-103: Methods for characterizing commensurate and incommensurate magnetic structures			CHAIR	0	Francoise Damay	1252
27-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-103: Methods for characterizing commensurate and incommensurate magnetic structures	817	Conventional and unconventional studies of magnetic structures with x-rays	Oral 30 mins	1	Prof Stephen Patrick Collins	1204
27-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-103: Methods for characterizing commensurate and incommensurate magnetic structures	844	Striped Magnetic Ground State on an Ideal S=2 Kagomé Lattice	Oral 30 mins	2	Prof Chris D Ling	1231
27-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-103: Methods for characterizing commensurate and incommensurate magnetic structures	851	Orbital ordering and structural distortions in vanadium spinels	Oral 30 mins	3	Mr Alexander J. Browne	1234
27-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-103: Methods for characterizing commensurate and incommensurate magnetic structures	1477	Structure property relationships in magnetocaloric materials	Oral 30 mins	4	Dr Karen Friese	1678
27-08-2017	1455-1730	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-103: Methods for characterizing commensurate and incommensurate magnetic structures	1055	Helical magnetic structure in cubic chiral crystal Pr <sub>5</sub> Ru <sub>3</sub> Al <sub>2</sub>	Oral 30 mins	5	Dr Daisuke Okuyama	1355

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27-08-2017	1455-1730	MR 1.05	Special Activities	MS-104: Synchrotron measurement in conservation and cultural heritage			CHAIR	0	Eric Dooryh�e	1701
27-08-2017	1455-1730	MR 1.05	Special Activities	MS-104: Synchrotron measurement in conservation and cultural heritage	733	Synchrotron-based micro-analyses of artistic materials at ID21, ESRF	Oral 30 mins	1	Dr Marine Cotte	1142
27-08-2017	1455-1730	MR 1.05	Special Activities	MS-104: Synchrotron measurement in conservation and cultural heritage	543	Deciphering Ceramic Workshops Practices in Classical Athens	Oral 30 mins	2	Dr Apurva Mehta	894
27-08-2017	1455-1730	MR 1.05	Special Activities	MS-104: Synchrotron measurement in conservation and cultural heritage	1413	$\mu$ XRD for the identification of pigments in cross-sections of paintings	Oral 30 mins	3	Dr Bernadette Fruehmann	1576
27-08-2017	1455-1730	MR 1.05	Special Activities	MS-104: Synchrotron measurement in conservation and cultural heritage	1393	Using neutron tomography to examine guitar strings	Oral 30 mins	4	Dr Alison Jeanine Edwards	1186
27-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-105: New instrumental developments for electron crystallography			CHAIR	0	Fu-Rong Chen	2396
27-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-105: New instrumental developments for electron crystallography			CHAIR	0	Pete Nellist	1269
27-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-105: New instrumental developments for electron crystallography	1795	Optimization of Automated electron Diffraction Tomography for challenging applications	Oral 30 mins	1	Prof Ute Kolb	1929
27-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-105: New instrumental developments for electron crystallography	1427	Electron Ptychographic Phase Imaging Using Fast Pixelated Detectors	Oral 30 mins	2	Dr Hao Yang	1650
27-08-2017	1455-1730	MR 1.06	Instrumentation techniques and/or Computation	MS-105: New instrumental developments for electron crystallography	1630	A new electron-counting detector for electron diffraction	Oral 30 mins	3	Dr Clemens Schulze-Briese	1369

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27-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-106: Functional materials on the nanoscale			CHAIR	0	Gregory Warr	2077
27-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-106: Functional materials on the nanoscale			CHAIR	0	U. S. Jeng	1825
27-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-106: Functional materials on the nanoscale	1126	Nanostructures from Self-Assembled Block Copolymer/Nanoparticle Mixtures	Oral 30 mins	1	Prof Bhanu Nandan	1444
27-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-106: Functional materials on the nanoscale	1604	Probing the pathways of nanoscale self-assembly	Oral 30 mins	2	Dr Theyencheri Narayanan	1755
27-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-106: Functional materials on the nanoscale	1987	Structure and Dynamics of Conjugated Polymers from Scattering and Simulations	Oral 30 mins	3	Prof Lilo Danielle Pozzo	2162
27-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-106: Functional materials on the nanoscale	913	Nanostructures in GeTe-rich materials: substitution, defects, thermoelectricity	Oral 15 mins	4	Prof Oliver Oeckler	1282
27-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-106: Functional materials on the nanoscale	164	Nano scale structural analyses on Turkey/Taiwan originated spiders' cocoons	Oral 15 mins	5	Prof Semra Ide	482
27-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-106: Functional materials on the nanoscale	1265	Inorganic Super-Fullerenes: Remarkable Versatility For Nano-confined Functionalization	Oral 15 mins	6	Dr Somenath Garai	1553
27-08-2017	1455-1730	MR 2.01	Materials and Minerals	MS-106: Functional materials on the nanoscale	169	Imaging of Nanoscale Molecular Order in the Cybotactic Nematic Phase	Oral 15 mins	7	Dr Venkatesh Gude	209
27-08-2017	1455-1730	MR 2.02	Special Activities	MS-107: Robust programming for CIF, NeXus, and related file structures			CHAIR	0	John Bollinger	563
27-08-2017	1455-1730	MR 2.02	Special Activities	MS-107: Robust programming for CIF, NeXus, and related file structures	1768	Driving universal data format input and translation using CIF dictionaries	Oral 30 mins	1	Dr James Reginald Hester	1121
27-08-2017	1455-1730	MR 2.02	Special Activities	MS-107: Robust programming for CIF, NeXus, and related file structures	906	Maintaining and obtaining maximum value from a CIF publication archive	Oral 30 mins	2	Mr Brian McMahon	1283
27-08-2017	1455-1730	MR 2.02	Special Activities	MS-107: Robust programming for CIF, NeXus, and related file structures	633	CIF1 to CIF2: Lessons learned in the development of Jmol	Oral 30 mins	3	Prof Robert Mark Hanson	678

Date	Time	Hall	Theme	Microsymposium (MS)	ABS-Num.	Abstract Title	Presentation Type	Sequence	Chair/Author Name	Database ID
27-08-2017	1455-1730	MR 2.02	Special Activities	MS-107: Robust programming for CIF, NeXus, and related file structures	962	PDBx/mmCIF: The Foundation for the wwPDB OneDep System	Oral 30 mins	4	Dr John Westbrook	805
27-08-2017	1455-1730	MR 2.02	Special Activities	MS-107: Robust programming for CIF, NeXus, and related file structures	1314	Fast and flexible CIF processing with the CIF API	Oral 15 mins	5	Dr John C. Bollinger	563
27-08-2017	1455-1730	MR 2.02	Special Activities	MS-107: Robust programming for CIF, NeXus, and related file structures	902	Software for Processing High-Data-Rate MX in CIF and NeXus/HDF5	Oral 15 mins	6	Dr Herbert Jacob Bernstein	407
27-08-2017	1455-1730	MR 2.02	Materials and Minerals	MS-108: Charge and spin density in molecular and supramolecular magnets			CHAIR	0	Claude Lecomte	667
27-08-2017	1455-1730	MR 2.02	Materials and Minerals	MS-108: Charge and spin density in molecular and supramolecular magnets	516	joint-refinement of spin and charge densities of organic radicals:	Oral 30 mins	1	Prof Mohamed Souhassou	653
27-08-2017	1455-1730	MR 2.02	Materials and Minerals	MS-108: Charge and spin density in molecular and supramolecular magnets	720	Charge density and magnetic anisotropy of Dy-based single molecule magnet	Oral 30 mins	2	Dr Jacob Overgaard	1128
27-08-2017	1455-1730	MR 2.02	Materials and Minerals	MS-108: Charge and spin density in molecular and supramolecular magnets	1390	Charge and Spin Density Study of Ni(III) dithiolate complex	Oral 30 mins	3	Dr Jozef Kozisek	1363
28-08-2017	1030-1305	Hall 4	Special Activities	MS-109: CryoEM: Method of the decade			CHAIR	0	Richard Henderson	77
28-08-2017	1030-1305	Hall 4	Special Activities	MS-109: CryoEM: Method of the decade			CHAIR	0	Samar Hasnain	313
28-08-2017	1030-1305	Hall 4	Special Activities	MS-109: CryoEM: Method of the decade	1981	Single particle cryo-EM of membrane proteins in lipid nanodisc	Oral 30 mins	1	Prof Yifan Cheng	2152
28-08-2017	1030-1305	Hall 4	Special Activities	MS-109: CryoEM: Method of the decade	2014	cisTEM: User-friendly software for single-particle image processing	Oral 30 mins	2	Dr Nikolaus Grigorieff	145
28-08-2017	1030-1305	Hall 4	Special Activities	MS-109: CryoEM: Method of the decade	2019	A new method for vitrifying samples for cryoEM	Oral 30 mins	3	Dr Bridget Carragher	2213
28-08-2017	1030-1305	Hall 4	Special Activities	MS-109: CryoEM: Method of the decade	2015	CryoEM of membrane protein complexes	Oral 30 mins	4	Prof Werner Kuehlbrandt	2159
28-08-2017	1030-1305	Hall 4	Special Activities	MS-109: CryoEM: Method of the decade	2027	Cryo EM studies of protein aggregation and disaggregation	Oral 30 mins	5	Prof Helen Saibil	2225

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28-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-110: Phase transition in alloys and molecular solids			CHAIR	0	Kinga Suwinska	260
28-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-110: Phase transition in alloys and molecular solids			CHAIR	0	Anthony Linden	96
28-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-110: Phase transition in alloys and molecular solids	850	Phase changes and chemical reactions in molecular crystals	Oral 30 mins	1	Prof Lawrence Rocco Falvello	623
28-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-110: Phase transition in alloys and molecular solids	514	Materials studies by the Bilbao Crystallographic Server	Oral 30 mins	2	Prof Mois Ilia Aroyo	929
28-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-110: Phase transition in alloys and molecular solids	1130	Competing bcc $\beta \rightarrow$ hcp $\alpha$ phase transformations in Ti-1Mo alloy	Oral 30 mins	3	Dr Sabeena M	1441
28-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-110: Phase transition in alloys and molecular solids	630	Mystique world of acrobatic molecular crystals	Oral 30 mins	4	Prof Zeljko Skoko	1049
28-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-110: Phase transition in alloys and molecular solids	267	Multiscale structural view of phase transitions in spin-crossover molecular solids	Oral 15 mins	5	Prof Philippe Guionneau	650
28-08-2017	1030-1305	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-110: Phase transition in alloys and molecular solids	1216	Phase transition study of Ag doped Ge <sub>2</sub> Sb <sub>2</sub> Te <sub>5</sub> thin films	Oral 15 mins	6	Mr Palwinder Singh	493
28-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-111: Structural chemistry at non-ambient conditions			CHAIR	0	Dave Billing	1031
28-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-111: Structural chemistry at non-ambient conditions			CHAIR	0	Manuel Fernandez	2016
28-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-111: Structural chemistry at non-ambient conditions	1591	Under pressure to react – acetylenedicarboxylic acid polymerisation	Oral 30 mins	1	Dr Iain Douglas Hood Oswald	1741
28-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-111: Structural chemistry at non-ambient conditions	1493	New guest accessible space under gas pressure	Oral 30 mins	2	Dr Vincent Joseph Smith	1680
28-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-111: Structural chemistry at non-ambient conditions	465	A High Pressure Study of Two Polymorphs of C <sub>60</sub> -2S8	Oral 30 mins	3	Dr Christine M. Beavers	864

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28-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-111: Structural chemistry at non-ambient conditions	1210	New developments using the "in situ" crystallization with a CO2-laser	Oral 30 mins	4	Dr Jordi Benet Buchholz	847
28-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-111: Structural chemistry at non-ambient conditions	1207	Geometry limitation-free HT device for in situ/operando SCXRD	Oral 15 mins	5	Dr Michele Zema	1493
28-08-2017	1030-1305	Hall 6	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-111: Structural chemistry at non-ambient conditions	1745	Weak donor-acceptor intermolecular interactions under pressure: the NO <sub>2</sub> ...NO <sub>2</sub> case.	Oral 15 mins	6	Mr Fabio Montisci	1882
28-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-112: Laboratory sources vs. large scale facilities for charge density studies			CHAIR	0	Regine Herbst-Irmer	348
28-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-112: Laboratory sources vs. large scale facilities for charge density studies			CHAIR	0	Jacob Overgaard	1128
28-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-112: Laboratory sources vs. large scale facilities for charge density studies	293	Accurate Charge Densities from Powder X-Ray Diffraction	Oral 30 mins	1	Dr Mads Ry Vogel Jørgensen	691
28-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-112: Laboratory sources vs. large scale facilities for charge density studies	352	YTiO3 charge densities: comparison of synchrotron / laboratory diffraction data	Oral 30 mins	2	Dr Nicolas Claiser	652
28-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-112: Laboratory sources vs. large scale facilities for charge density studies	1810	Charge-density studies in small molecules and proteins: Sources and detectors	Oral 30 mins	3	Dr Parthapratim Munshi	1495
28-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-112: Laboratory sources vs. large scale facilities for charge density studies	378	Precision and Accuracy of Single Crystal X-Ray Results	Oral 30 mins	4	Prof Krzysztof Wozniak	787
28-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-112: Laboratory sources vs. large scale facilities for charge density studies	995	High resolution charge density of metal hexaborides.	Oral 15 mins	5	Prof Eiji Nishibori	1315
28-08-2017	1030-1305	MR 1.01 - 1.03	Instrumentation techniques and/or Computation	MS-112: Laboratory sources vs. large scale facilities for charge density studies	1076	Charge density study of van der Waals-layered MoS <sub>2</sub> and TiS <sub>2</sub>	Oral 15 mins	6	Dr Hidetaka Kasai	1041

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28-08-2017	1030-1305	MR 1.05	Special Activities	MS-113: Anticipating the Harvest: Post IYCr			CHAIR	0	Jean-Paul Ngome Abiag a	783
28-08-2017	1030-1305	MR 1.05	Special Activities	MS-113: Anticipating the Harvest: Post IYCr			CHAIR	0	Michele Zema	1493
28-08-2017	1030-1305	MR 1.05	Special Activities	MS-113: Anticipating the Harvest: Post IYCr	372	Crystallography for sustainable development: UNESCO's role and strategy	Oral 30 mins	1	Dr Juste Jean Paul Ngome Abiaga	783
28-08-2017	1030-1305	MR 1.05	Special Activities	MS-113: Anticipating the Harvest: Post IYCr	1234	Crystallography and scientific research in Africa: role of ICSU ROA	Oral 30 mins	2	Dr Daniel Nyanganyura	1531
28-08-2017	1030-1305	MR 1.05	Special Activities	MS-113: Anticipating the Harvest: Post IYCr	943	The First Protein Crystallography Project in Jordan	Oral 30 mins	3	Dr Areej Abuhammad	1265
28-08-2017	1030-1305	MR 1.05	Special Activities	MS-113: Anticipating the Harvest: Post IYCr	275	The Africa Initiative and the PanAfrican Conferences on crystallography PCCr	Oral 15 mins	4	Prof Claude Edouard Paul Lecomte	667
28-08-2017	1030-1305	MR 1.05	Special Activities	MS-113: Anticipating the Harvest: Post IYCr	916	Open Data in the emerging 21st-century scientific world	Oral 15 mins	5	Mr Brian McMahon	1283
28-08-2017	1030-1305	MR 1.05	Special Activities	MS-113: Anticipating the Harvest: Post IYCr	985	Post IYCr in Latin America: scientific, academic and outreach activities	Oral 10 mins	6	Dr Diego Germán Lamas	1323
28-08-2017	1030-1305	MR 1.05	Special Activities	MS-113: Anticipating the Harvest: Post IYCr	462	The road to the Association of Albanian Crystallographers	Oral 10 mins	7	Prof Bujar Dida	810
28-08-2017	1030-1305	MR 1.05	Special Activities	MS-113: Anticipating the Harvest: Post IYCr	1250	Bangladesh Crystallographic Association (BCA) – its formation and activities.	Oral 10 mins	8	Prof Altaf Hussain	359
28-08-2017	1030-1305	MR 1.06	Special Activities	MS-114: Crystallography and cultural heritage: From microsampling to noninvasive techniques			CHAIR	0	Manfred Schreiner	2168
28-08-2017	1030-1305	MR 1.06	Special Activities	MS-114: Crystallography and cultural heritage: From microsampling to noninvasive techniques			CHAIR	0	Serge Cohen	2076
28-08-2017	1030-1305	MR 1.06	Special Activities	MS-114: Crystallography and cultural heritage: From microsampling to noninvasive techniques	767	Multimodal investigation of Pb- and As-based pigment degradation	Oral 30 mins	1	Prof Koen Henri Janssens	1168
28-08-2017	1030-1305	MR 1.06	Special Activities	MS-114: Crystallography and cultural heritage: From microsampling to noninvasive techniques	1226	X-ray powder diffraction structural studies of lithol red pigments	Oral 30 mins	2	Prof Wieslaw Lasocha	1122

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28-08-2017	1030-1305	MR 1.06	Special Activities	MS-114: Crystallography and cultural heritage: From microsampling to noninvasive techniques	533	Red/yellow pigments in Pompeii and Herculaneum: which is which?	Oral 30 mins	3	Prof Gilberto Artioli	936
28-08-2017	1030-1305	MR 1.06	Special Activities	MS-114: Crystallography and cultural heritage: From microsampling to noninvasive techniques	1572	Potential of forensic analysis of multicomponent samples	Oral 15 mins	4	Dr Marek Kotrly	1727
28-08-2017	1030-1305	MR 1.06	Special Activities	MS-114: Crystallography and cultural heritage: From microsampling to noninvasive techniques	1103	Comprehensive studies of cultural heritage objects in NRC Kurchatov Institute	Oral 15 mins	5	Dr Roman Senin	1274
28-08-2017	1030-1305	MR 1.06	Special Activities	MS-114: Crystallography and cultural heritage: From microsampling to noninvasive techniques	1688	Characterization of ancient Harappan faience bangles	Oral 2 mins	6	Prof Gilberto Artioli	936
28-08-2017	1030-1305	MR 1.06	Special Activities	MS-114: Crystallography and cultural heritage: From microsampling to noninvasive techniques	1413	$\mu$ XRD for the identification of pigments in cross-sections of paintings	Oral 2 mins	7	Dr Bernadette Fruehmann	1576
28-08-2017	1030-1305	MR 1.06	Special Activities	MS-114: Crystallography and cultural heritage: From microsampling to noninvasive techniques	1401	In-situ and time-lapse XRD as tools for atmospheric corrosion research	Oral 2 mins	8	Dr Rita Wiesinger	1558
28-08-2017	1030-1305	MR 1.06	Special Activities	MS-114: Crystallography and cultural heritage: From microsampling to noninvasive techniques	1336	On the grounds of icons from National Museum in Krakow	Oral 2 mins	9	Dr Alicja Rafalska-Lasocha	1127
28-08-2017	1030-1305	MR 1.06	Special Activities	MS-114: Crystallography and cultural heritage: From microsampling to noninvasive techniques	263	Verifying the reliability of historical sources through an archaeometric study	Oral 2 mins	10	Prof Simona Quartieri	117
28-08-2017	1030-1305	MR 1.06	Special Activities	MS-114: Crystallography and cultural heritage: From microsampling to noninvasive techniques	1542	Electron microscopy methods in studies of Archaeological Objects.	Oral 2 mins	11	Ms Natalia Kolobylna	1162



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28-08-2017	1030-1305	MR 2.01	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-115: Polymorphism and structural transformations in crystalline materials			CHAIR	0	Marijana Đaković	635
28-08-2017	1030-1305	MR 2.01	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-115: Polymorphism and structural transformations in crystalline materials			CHAIR	0	Koichi Momma	772
28-08-2017	1030-1305	MR 2.01	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-115: Polymorphism and structural transformations in crystalline materials	1404	Compressed interactions and properties of methyl-amine polymorphs	Oral 30 mins	1	Prof Andrzej Katrusiak	1634
28-08-2017	1030-1305	MR 2.01	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-115: Polymorphism and structural transformations in crystalline materials	1144	The high-temperature phases of L-phenylalanine	Oral 30 mins	2	Prof Carl Henrik Görbitz	1461
28-08-2017	1030-1305	MR 2.01	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-115: Polymorphism and structural transformations in crystalline materials	991	Unusual polymorphs of thymine	Oral 30 mins	3	Dr Susanta Kumar Nayak	923
28-08-2017	1030-1305	MR 2.01	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-115: Polymorphism and structural transformations in crystalline materials	927	Two-dimensional polymers: From monomer to polymer crystals and back	Oral 30 mins	4	Mr Gregor Hofer	706
28-08-2017	1030-1305	MR 2.01	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-115: Polymorphism and structural transformations in crystalline materials	1298	Template Induced Targeted Crystallisation of Computationally Predicted Polymorphs.	Oral 15 mins	5	Dr Vijay Kumar Srirambhatla	1569
28-08-2017	1030-1305	MR 2.01	Crystal Engineering of Organic & Pharmaceutical Compounds	MS-115: Polymorphism and structural transformations in crystalline materials	1952	Indentation plasticity of molecular crystals: Loading rate sensitivity studies	Oral 15 mins	6	Dr Kiran Mangalampalli	2098

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28-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-119: Interactions in solids under stress			CHAIR	0	Boris Zakharov	1385
28-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-119: Interactions in solids under stress			CHAIR	0	Shanti Deemyad	1994
28-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-119: Interactions in solids under stress	281	High-pressure transformation of MAPbI <sub>3</sub> : role of the noble-gas medium	Oral 30 mins	1	Dr Alla Arakcheeva	503
28-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-119: Interactions in solids under stress	1006	Emerging Challenges in High Pressure Neutron Scattering	Oral 30 mins	2	Dr Antonio M. dos Santos	1344
28-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-119: Interactions in solids under stress	380	Binding guest molecules to frameworks: pressure-induced chemisorption in breathing MOFs	Oral 30 mins	3	Dr Arianna Lanza	620
28-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-119: Interactions in solids under stress	836	Development of time-resolved x-ray acoustic method of investigation of crystals	Oral 15 mins	4	Mr Anton Targonskiy	1224
28-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-119: Interactions in solids under stress	1499	Complexity in supramolecular analogues of frustrated magnets at high pressure	Oral 15 mins	5	Dr Andrew Brian Cairns	1606
28-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-119: Interactions in solids under stress	874	Structure–property relationships in multiferroic metal–formate frameworks under pressure	Oral 15 mins	6	Dr Ines Emily Collings	1254
28-08-2017	1455-1730	Hall 5	Crystal Engineering of MOFs & Open Framework Compounds	MS-119: Interactions in solids under stress	1322	HP-HT behavior of urea, a precursor to photocatalytic materials	Oral 15 mins	7	Dr Kamil Filip Dziubek	1549
28-08-2017	1455-1730	MR 1.05	Materials and Minerals	MS-122: Crystallography of materials for energy			CHAIR	0	Oliver Oeckler	1282
28-08-2017	1455-1730	MR 1.05	Materials and Minerals	MS-122: Crystallography of materials for energy			CHAIR	0	Artem Abakumov	838
28-08-2017	1455-1730	MR 1.05	Materials and Minerals	MS-122: Crystallography of materials for energy	497	Thermally and Electrochemically Driven Topotactical Transformations in Sodium Layered Oxides	Oral 30 mins	1	Dr Marie Guignard	907
28-08-2017	1455-1730	MR 1.05	Materials and Minerals	MS-122: Crystallography of materials for energy	750	Solar cell structure at micro- and nanoscale through TEM	Oral 30 mins	2	Prof Joke Hadermann	1159
28-08-2017	1455-1730	MR 1.05	Materials and Minerals	MS-122: Crystallography of materials for energy	1307	Disorder in LiMn <sub>2</sub> -xTi <sub>x</sub> O <sub>4</sub> determined from combined diffraction and XAS studies	Oral 30 mins	3	Dr Siegbert Schmid	1514

Date	Time	Hall	Theme	Microsymposium (MS)	ABS-Num.	Abstract Title	Presentation Type	Sequence	Chair/Author Name	Database ID
28-08-2017	1455-1730	MR 1.05	Materials and Minerals	MS-122: Crystallography of materials for energy	1283	Neutron diffraction studies of oxygen disorder in Nd <sub>2</sub> NiO <sub>4+d</sub>	Oral 30 mins	4	Mr Sumit Ranjan Maity	119
28-08-2017	1455-1730	MR 1.05	Materials and Minerals	MS-122: Crystallography of materials for energy	433	Intrusion-extrusion of electrolytic solutions in zeolites for energy storage	Oral 15 mins	5	Prof Rossella Arletti	792
28-08-2017	1455-1730	MR 1.05	Materials and Minerals	MS-122: Crystallography of materials for energy	314	Ion-Transport Phenomena and Anomalous Transformations In Strontium Uranium Oxides.	Oral 15 mins	6	Mr Gabriel Lynch Murphy	713
28-08-2017	1455-1730	MR 1.06	Physical and/or Fundamental	MS-123: Magnetic structures at extreme conditions			CHAIR	0	Oleksander Prokhnenko	649
28-08-2017	1455-1730	MR 1.06	Physical and/or Fundamental	MS-123: Magnetic structures at extreme conditions			CHAIR	0	Konstantin Kamenev	Not in database
28-08-2017	1455-1730	MR 1.06	Physical and/or Fundamental	MS-123: Magnetic structures at extreme conditions	614	Neutron Diffraction Experiments in Pulsed Magnetic Fields	Oral 30 mins	1	Prof Hiroyuki Nojiri	1033
28-08-2017	1455-1730	MR 1.06	Physical and/or Fundamental	MS-123: Magnetic structures at extreme conditions	190	What can we learn from not so high pressure physics?	Oral 30 mins	2	Dr Andrey Podlesnyak	427
28-08-2017	1455-1730	MR 1.06	Physical and/or Fundamental	MS-123: Magnetic structures at extreme conditions	599	Neutron studies on high pressure A-site manganites.	Oral 30 mins	3	Dr Angel M Arevalo Lopez	1020
28-08-2017	1455-1730	MR 1.06	Physical and/or Fundamental	MS-123: Magnetic structures at extreme conditions	1383	High pressure structural and electronic transitions in lithium ferrites	Oral 30 mins	4	Dr Samar Layek	1593
28-08-2017	1455-1730	MR 1.06	Physical and/or Fundamental	MS-123: Magnetic structures at extreme conditions	2054	Modulating magnetic anisotropy in coordination complexes using hydrostatic pressure	Oral 30 mins	5	Dr Gavin Craig	2275

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28-08-2017	1455-1730	MR 2.01	Physical and/or Fundamental	MS-124: Beyond conventional topological analysis of electron density			CHAIR	0	Bernardo Rodrigues	957
28-08-2017	1455-1730	MR 2.01	Physical and/or Fundamental	MS-124: Beyond conventional topological analysis of electron density			CHAIR	0	Julia Contreras	931
28-08-2017	1455-1730	MR 2.01	Physical and/or Fundamental	MS-124: Beyond conventional topological analysis of electron density	1195	Insights on spin density delocalization/polarization mechanisms through the Source Function	Oral 30 mins	1	Dr Carlo Gatti	1501
28-08-2017	1455-1730	MR 2.01	Physical and/or Fundamental	MS-124: Beyond conventional topological analysis of electron density	238	Libraries of Extremely Localized Molecular Orbitals	Oral 30 mins	2	Dr Alessandro Genoni	410
28-08-2017	1455-1730	MR 2.01	Physical and/or Fundamental	MS-124: Beyond conventional topological analysis of electron density	1186	From molecules to materials, efficient crystal engineering of polar systems	Oral 30 mins	3	Dr Marlena Gryl	1228
28-08-2017	1455-1730	MR 2.01	Physical and/or Fundamental	MS-124: Beyond conventional topological analysis of electron density	881	Electron pairing over domains	Oral 30 mins	4	Dr Miroslav Kohout	1256
28-08-2017	1455-1730	MR 2.01	Physical and/or Fundamental	MS-124: Beyond conventional topological analysis of electron density	1127	Electric fields in crown ether complexation with neutral molecules	Oral 15 mins	5	Mr Mingwen Shi	515
28-08-2017	1455-1730	MR 2.01	Physical and/or Fundamental	MS-124: Beyond conventional topological analysis of electron density	1016	Experimental charge densities of nucleobase chlorides from intermolecular interaction perspective	Oral 15 mins	6	Dr Paulina M. Dominiak	532

Date	Time	Hall	Theme	Microsymposium (MS)	ABS-Num.	Abstract Title	Presentation Type	Sequence	Chair/Author Name	Database ID
28-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-125: Small-Angle Scattering data formats, standards and repositories			CHAIR	0	Cy Jeffries	157
28-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-125: Small-Angle Scattering data formats, standards and repositories			CHAIR	0	Manfred Roessle	2102
28-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-125: Small-Angle Scattering data formats, standards and repositories	1288	Validation of biological small-angle scattering data and models in SASBDB	Oral 30 mins	1	Dr Alexey Kikhney	509
28-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-125: Small-Angle Scattering data formats, standards and repositories	1977	Small-Angle Scattering Data Representation in SASCIF and Integrative/Hybrid Methods Dictionary	Oral 30 mins	2	Dr Brinda Vallat	1619
28-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-125: Small-Angle Scattering data formats, standards and repositories	974	NXcanSAS: standard to store reduced SAS data of any dimension	Oral 30 mins	3	Dr Pete R Jemian	1324
28-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-125: Small-Angle Scattering data formats, standards and repositories	2004	Small-angle scattering standards and absolute intensity calibration	Oral 30 mins	4	Dr Andrew John Allen	1347
28-08-2017	1455-1730	MR 2.02	Physical and/or Fundamental	MS-125: Small-Angle Scattering data formats, standards and repositories	1769	Publication Guidelines for Biomolecular Small-Angle Scattering: A Community Driven Effort	Oral 30 mins	5	Prof Jules Mitchell Guss	200