

Morning Session 8:30-9:30**A-05MH (KN 28)****KN28(C10) | Tom L Blundell:**

Structural pharmacology and drug discovery: Exploring biological and chemical space

Chair: **Tsuyoshi Inoue**

F-12CH (KN 29)**KN29(C10) | Mohamed Eddaoudi:**

Metal-organic materials: Strategies functional porous materials

Chair: **Sue-Lein Wang**

D-1003 (KN 30)**KN30(C11) | Paolo G Radaelli:**

Atoms and spins in novel multiferroics: A new twist to an old relation

Chair: **Juan Rodriguez-Carvajal**

Afternoon Session 17:30-18:30**A-05MH (KN 31)****KN31(C11) | Vincent Villeret:**

Structure of the FhaC translocation pore : Insights into transport across the bacterial membrane

Chair: **Brian W. Matthews**

F-12CH (KN 32)**KN32(C11) | Michael Zaworotko:**

Crystal engineering of co-crystals and their relevance to pharmaceuticals and solid-state chemistry

Chair: **Nair Rodriguez-Hornedo**

D-1003 (KN 33)**KN33(C12) | An-Pang Tsai:**

Quasicrystals structures properties and applications

Chair: **Walter Steurer**

Friday, August 29 - Morning - Microsymposia

Friday, August 29 - Morning - Microsymposia

Time	A-05MH (MS 71)	F-12CH (MS 72)	D-1003 (MS 73)
9:55-10:00 Opening Remarks	Biophysical techniques for detecting ligand binding to pharmaceutical targets Chairs: R. E. Hubbard, Y. Kawakami	Micro-SAXS for nanoscience and medicine Chairs: P. Fratzl, J. Doucet	Structure-functions relationships of MOF Chairs: M. Eddaudi, S. L.James
10:00-10:30	MS.71.1(C121) A. Ruf: X-ray structural analysis and biophysical assays in drug discovery	MS.72.1(C123) T. Pfohl: Combining microfluidics with micro-SAXS for studies of the dynamics of DNA compaction	MS.73.1(C124) R. Matsuda: Guest-responsive structures and properties of porous coordination polymers
10:30-11:00	MS.71.2(C121) S. Akashi: Studies of protein-protein and protein-RNA complexes by mass spectrometry	MS.72.2(C123) M. Foldvari: Application of SWAXS in nanomedicine: Characterizing nanoparticles and their interaction with skin	MS.73.2(C125) M. J. Rosseinsky: <i>In-situ</i> reactivity and selective chiral sorption in metal-organic frameworks
11:00-11:30	MS.71.3(C122) J. Murray: Characterising protein-ligand binding in support of structure-based drug discovery	MS.72.3(C123) F. Artzner: Peptidic nanotubes : From drug release to glass nanowires	MS.73.3(C125) L. J. Barbour: Porosity in flexible metal-organic systems
11:30-12:00	MS.71.4(C122) L. Gabison: Mechanism of the cofactor-less urate oxidase: X-ray structures with molecular oxygen or cyanide.	MS.72.4(C124) D. Viterbo: A mesoporous pattern created by nature: A SAXS and micro-SAXS study	MS.73.4(C125) G. Zhu: The synthesis and structure of multifunctional metal-organic frameworks
12:00-12:30	MS.71.5(C122) L. N. Johnson: Flavopiridol binding to P-TEFb (CDK9/cyclin T1)	MS.72.5(C124) Y. Nozue: Deformation behavior of drawn polymer spherulite studied by simultaneous micro SAXS-WAXS and POM	MS.73.5(C125) N. Lock: Elucidating negative thermal expansion in metal-organic frameworks

C-1001, 2 (MS 74)	G-1202 (MS 75)	B-05SH (MS 76)	E-1009 (MS 77)
Multiferroic materials Chairs: T. Kimura, L. Pinsard-Gaudart	Charge, spin and momentum density studies in material science Chairs: B. Gillon, P. Macchi	Diffractive imaging Chairs: F. Chen, H. Faulkner	Diffuse scattering in partially ordered/disordered systems Chairs: H. Abe, C. Branton
MS.74.1(C126) Y. Noda: Magnetic and crystal structure in connection with ferroelectric properties of multiferroic RMn ₂ O ₅	MS.75.1(C127) W. Scherer: Electron localization phenomena in complex carbides of rare earth and transition metals	MS.76.1(C129) K. A. Nugent: Coherent diffractive imaging: A new tool for high resolution X-ray imaging	MS.77.1(C131) R. Welberry: Diffuse scattering as a probe of local structure
MS.74.2(C126) M. Kenzelmann: Ferroelectricity from magnetic order	MS.75.2(C128) J. Kozisek: Study of electronic structure of tetrakis(μ_2 -Acetato)-diaqua-di-copper(II) complex	MS.76.2(C129) U. J. Weierstall: Diffractive imaging and serial crystallography	MS.77.2(C131) M. Takahashi: Magnetic short-range order in Pt-rich Pt-Mn alloys
MS.74.3(C126) D. N. Argyriou: Function from frustration in modern multiferroics	MS.75.3(C128) P. Munshi: Estimation of optical properties from wavefunction fitting of X-ray diffraction data	MS.76.3(C130) R. V. Dronyak: Electron diffractive imaging of the MgO nanoparticle: Towards atomic-resolution	MS.77.3(C131) S. M. P. Francoual: Phason diffuse scattering in the icosahedral quasicrystalline phases Zn-X-Sc, X = Co, Ag, Mg
MS.74.4(C127) F. H. Damay: Crystal and magnetic structures of frustrated antiferromagnet CuCrO ₂	MS.75.4(C128) J. Campo: Magnetic interactions in thiazyl-based magnets: The role of the charge and spin densities	MS.76.4(C130) C. Giannini: Coherent X-ray diffraction imaging of non periodic single objects	MS.77.4(C131) T. Weber: 3D-PDF analysis of single crystal diffuse scattering on the example of disordered quasicrystals
MS.74.5(C127) J. B. Claridge: Frustration of magnetic and ferroelectric long-range order in Bi ₂ Mn _{4/3} Ni _{2/3} O ₆	MS.75.5(C129) M. Ito: Observation of spin densities by the X-ray magnetic diffraction	MS.76.5(C130) K. Kawahara: Beam divergence in electron diffractive imaging	MS.77.5(C132) S. Haas: Nanostructure of silver-free photochromic glasses studied by anomalous small angle X-ray scattering

Friday, August 29 - Afternoon - Microsymposia

Time	A-05MH (MS 78)	F-12CH (MS 79)	D-1003 (MS 80)
14:45-14:50 Opening Remarks	Crystallization of membrane proteins Chairs: E. Pebay-Peroula, S. Yoshikawa	Motion in macromolecular machines Chairs: M. Rossmann, H. Wu	Understanding and controlling polymorphism Chairs: S. M. Reutzel-Edens, U. Rychlewska
14:50-15:20	MS.78.1(C132) J-L. Popot: Can amphipols be used to crystallize membrane proteins?	MS.79.1(C134) K. Namba: Molecular mechanisms of self-assembly and motion of the bacterial flagellum	MS.80.1(C135) J. Bernstein: Understanding and controlling polymorphism
15:20-15:50	MS.78.2(C132) C. Toyoshima: Crystallisation of the calcium pump of skeletal muscle sarcoplasmic reticulum	MS.79.2(C134) V. B. Rao: Mechanism of DNA packaging in bacteriophage T4	MS.80.2(C135) K. Fujii: Dehydration process of lisinopril, investigated by <i>ab initio</i> powder crystal structure analysis
15:50-16:20	MS.78.3(C133) T. Kouyama: Crystallization of visual pigments and archaeal rhodopsins	MS.79.3(C134) J. Lowe: DNA translocation by hexameric FtsK	MS.80.3(C136) L. Yu: What do polymorphs teach us about crystal nucleation and growth?
16:20-16:50	MS.78.4(C133) S. Maeda: X-ray structure of human gap junction channel	MS.79.4(C134) C. V. Stauffacher: Crystallographic snapshots of the enzyme mechanisms of HMG-CoA reductase and HMG-CoA synthase	MS.80.4(C136) E. J. Chan: Modeling single crystal diffuse scattering on polymorphs of the drug benzocaine
16:50-17:20	MS.78.5(C133) A. May: Diffraction-capable microfluidic crystallization chips for screening and structure determination	MS.79.5(C135) D. Luo: Crystal structure of the NS3 protease-helicase from Dengue virus	MS.80.5(C136) S. L. Price: Computed crystal energy landscapes as an aid to understanding polymorphism

Friday, August 29 - Afternoon - Microsymposia

C-1001, 2 (MS 81)	G-1202 (MS 82)	B-05SH (MS 83)	E-1009 (MS 84)
New neutron sources Chairs: S. J. Kennedy, Y. Noda	Magnetic compton scattering Chairs: Y. Sakurai, H. Kawata	Femto-second diffraction: Time resolved studies Chairs: S. Techert, R. Feidenhans'l	Quasicrystals and related giant crystalline alloys Chairs: E. Abe, R. McGrath
MS.81.1(C137) B. J. Kennedy: Crystallography at the new Australian research reactor OPAL	MS.82.1(C138) N. Sakai: Momentum density of uncompensated electron spins measured by magnetic Compton scattering	MS.83.1(C140) J. Miao: Coherent diffraction microscopy: Present and future	MS.84.1(C141) F. Fleischer: Performance tests on iterative phase-retrieval methods in higher dimensions
MS.81.2(C137) C-H. Lee: Current situation of the cold neutron research facility project at HANARO	MS.82.2(C138) A. Bansil: Inelastic X-ray scattering as a powerful probe of correlation effects in materials	MS.83.2(C140) M. M. Nielsen: Time-resolved X-ray scattering of an electronically excited state in metal complexes in solution	MS.84.2(C141) K. Sugiyama: Approximant structures for the AlCo based decagonal phases
MS.81.3(C137) I. S. Anderson: SNS and HFIR: Breaking new ground	MS.82.3(C139) J. A. Duffy: Using magnetic Compton scattering to study Invar and spin-polarised materials	MS.83.3(C140) S. L. Johnson: Femtosecond X-ray crystallography of elemental solids: Coherent dynamics in bismuth and tellurium	MS.84.3(C142) V. Fournee: New phenomena in epitaxial growth: Solid films on quasicrystalline substrates
MS.81.4(C137) Y. Ikeda: An advanced pulse neutron source and scientific challenges at J-PARC	MS.82.4(C139) H. Kobayashi: Magnetic Compton scattering under high pressure	MS.83.4(C140) J. Cao: Electronic Grüneisen parameter and thermal expansion in ferromagnetic transition metals	MS.84.4(C142) T. Dotera: Mesoscopic quasicrystalline and Archimedean tilings in polymer alloys
MS.81.5(C138) C. Vettier: Progress for the european spallation source	MS.82.5(C139) N. Qureshi: Spin and magnetization density in the kagome staircase system $\text{Co}_3\text{V}_2\text{O}_8$	MS.83.5(C141) A. Foehlisch: Ultrafast electron dynamics excited and probed with X-rays	MS.84.5(C142) M. De Boissieu: Atomic simulation and lattice dynamics of the ZnMgSc icosahedral quasicrystal