

Memo

Morning Session 8:30-9:30

A-05MH (KN 10)

KN10(C5) | Zihe Rao:
Structural biology studies of the avian influenza H5N1 virus

Chair: **Jack Johnson**

F-12CH (KN 11)

KN11(C5) | Tim White:
The crystallochemical basis of synthetic mineral immobilisation technologies

Chair: **Giovanni Ferraris**

D-1003 (KN 12)

KN12(C6) | Jian-Min Zuo:
Imaging of nanostructures at diffraction-limited resolution from electron diffraction patterns

Chair: **John C.H. Spence**

Afternoon Session 17:30-18:30

A-05MH (KN 13)

KN13(C6) | Yoshinori Fujiyoshi:
Structure and function of multifunctional channels

Chair: **Wah Chiu**

F-12CH (KN 14)

KN14(C6) | Claude E P Lecomte:
Experimental charge density modeling: Some frontier examples

Chair: **Philip Coppens**

D-1003 (KN 15)

KN15(C7) | Simon J. L. Billinge:
Nanostructure refinement and solution

Chair: **Takeshi Egami**

Time	A-05MH (MS 29)	F-12CH (MS 30)	D-1003 (MS 31)
9:55-10:00 Opening Remarks	Virus structure and antiviral strategies Chairs: J. Johnson, M. J. van Raaij	From minerals to materials Chairs: R. Hock, G. Ferey	Electric and magnetic properties of molecular crystals Chairs: M. Yamashita, A. Cornia
10:00-10:30	MS.29.1(C57) P. D. Kwong: X-ray crystallography and HIV vaccine design	MS.30.1(C59) G. L. W. Hart: Where are Nature's missing structures?	MS.31.1(C60) E. Coronado: Switching magnetic molecular materials
10:30-11:00	MS.29.2(C57) N. Verdagner: What we can learn from the structure of viral RNA-dependent RNA polymerases	MS.30.2(C59) N. N. Bramnik: High-voltage cathodes for Li-ion batteries: Metallophosphoolivines and manganese-based spinels	MS.31.2(C60) A. Kobayashi: Structures and physical properties of single-component molecular metals
11:00-11:30	MS.29.3(C58) F. A. Rey: Evolutionary links among viruses of different categories revealed by dsRNA virus capsid structures	MS.30.3(C59) J. B. Parise: Towards a better understanding of atomic arrangements in nano-minerals	MS.31.3(C61) V. Marvaud: Photoswitchable high spin molecules
11:30-12:00	MS.29.4(C58) J. E. Lee: Structure of the trimeric, prefusion Ebola virus GP complexed with an antibody from a human survivor	MS.30.4(C59) S. Schorr: Kesterite - an alternative absorber material for thin film solar cells	MS.31.4(C61) S. S. Khasanov: Structural aspects of magnetic transitions and high conductivity in ionic complexes of fullerenes
12:00-12:30	MS.29.5(C58) R. Hilgenfeld: (Re-)emerging viral diseases: How can structural biology support preparedness and response?	MS.30.5(C60) L. Bucio: Phase composition of mineral trioxide aggregate and its role on properties as biomaterial cement	MS.31.5(C61) Y. Ohgo: The spin-crossover triangle in the iron(III) porphyrinoids

C-1001, 2 (MS 32)	G-1202 (MS 33)	B-05SH (MS 34)	E-1009 (MS 35)
Nanostructure refinement and solution Chairs: C. Giannini, F. Matteucci	Liquids and amorphous systems at high pressure Chairs: M. Guthrie, Y. Katayama	Advanced electron microscopy Chairs: R. Holmestad, A. Kirkland	Combined XAFS and diffraction of inorganic structures Chairs: K. Asakura, A. Di Cicco
MS.32.1(C62) P. Juhas: Nanostructure investigations using atomic pair distribution function and other direct-space methods	MS.33.1(C63) S. A. Bonev: New liquid structures of alkali metals under pressure predicted from first principles theory	MS.34.1(C65) K. Suenaga: HR-TEM imaging of the carbon networks	MS.35.1(C66) D. T. Bowron: Comprehensive structural characterisation of local and bulk structure in disordered systems
MS.32.2(C62) A. Cervellino: Analysis of partially ordered (nano)materials through the Debye function method	MS.33.2(C63) M. G. Tucker: Total scattering studies of pressure induced amorphization	MS.34.2(C65) S. Stemmer: Image contrast in atomic resolution high-angle annular dark-field images	MS.35.2(C66) M. G. Newville: Developments of advanced XAFS analysis techniques with Ifeffit
MS.32.3(C62) Y. Andreev: Atomic arrangement in a nanotube from powder X-ray diffraction	MS.33.3(C64) K. Fuchizaki: Polyamorphism in tin tetraiodide	MS.34.3(C65) A. L. Bleloch: In aberration corrected STEM, shrinking some dimensions expands others	MS.35.3(C67) A. Michalowicz: Apparent mismatch between XAFS and XRD structure of crystalline and amorphous electrochromic WO ₃
MS.32.4(C63) C. F. Campana: The application of a molecular replacement approach to the refinement of a copper nanoball complex	MS.33.4(C64) K. Matsuda: Structural studies of expanded fluid alkali metals	MS.34.4(C65) O. Kamimura: Development of new electron diffraction microscope for diffractive imaging	MS.35.4(C67) A. Yoshiasa: High pressure and high temperature EXAFS and diffraction study of AgI
MS.32.5(C63) I. A. Vartanians: Coherent diffractive imaging of nanostructures at synchrotron and FEL sources	MS.33.5(C64) C. Sanloup: Structural transition in amorphous sulfur compressed up to 100 GPa	MS.34.5(C66) G. Botton: Applications of aberration-corrected TEM-STEM and high-resolution EELS in materials research	MS.35.5(C67) J. C. Hanson: <i>In situ</i> XRD and XAFS studies of oxidation/reduction and water gas shift reactions of Cu doped ceria

Time	A-05MH (MS 36)	F-12CH (MS 37)	D-1003 (MS 38)
14:45-14:50 Opening Remarks	Biological interests and biological electron microscopy Chairs: M. R. N. Murthy, K. Iwasaki	Crystal properties and bonding: What we really learn from accurate charge density studies and quantum calculations? Chairs: M. Spackman, K. Tanaka	Self-organization and self-assembly: From nucleation to crystal growth, from eutectics to photonic and liquid crystals, and from theory to application Chairs: D. Pawlak, P. Metrangolo
14:50-15:20	MS.36.1(C67) M. Wilmanns: Zooming into the overall architecture of the giant muscle protein titin	MS.37.1(C69) D. Stalke: Charge density based ligand design	MS.38.1(C71) L. Granasy: Phase field modeling of self-organized polycrystalline structures: Denrites, spherulites, eutectics
15:20-15:50	MS.36.2(C68) C. Sato: Ion channel structures by single particle analysis using EM: Sodium and TRP channels, IP3 receptor	MS.37.2(C69) D. Jayatilaka: Non-linear optical properties & structure determination by combining X-ray data and QM wavefunctions	MS.38.2(C71) Y. Waku: High temperature characteristics of unidirectionally solidified ceramic eutectics
15:50-16:20	MS.36.3(C68) T. Omura: The assembly process of the double-layered capsids of phytoreoviruses	MS.37.3(C70) D. Hashizume: Characterization of weak chemical bonds in highly strained and hypervalent compounds	MS.38.3(C71) G. G. Long: Nanoparticle halo formation around colloids in binary solutions
16:20-16:50	MS.36.4(C68) A. Goulet: A new virus structure: The nucleosome-like organization of the filamentous archaeal virus AFV1	MS.37.4(C70) C. Gatti: How and why elemental boron undergoes self charge transfer between 19 and 89 GPa	MS.38.4(C72) K. Itaya: Perfect single crystals of organic semiconductors prepared by crystallization from solutions
16:50-17:20	MS.36.5(C69) D. Suck: Structural studies of Holliday junction resolvases from bacteriophages, archaea and yeast	MS.37.5(C70) R. Orlando: Advances in quantum <i>ab initio</i> calculations with the CRYSTAL code	MS.38.5(C72) J. Nozawa: Self-assembled magnetite particles formed 4.6 billion years ago

C-1001, 2 (MS 39)	G-1202 (MS 40)	B-05SH (MS 41)	E-1009 (MS 42)
PDF/RDF analysis from pulsed-neutron and X-ray scattering Chairs: T. Egami, M. Tucker	Crystallography of planetary materials at extreme conditions Chairs: T. Yagi, J. Parise	Precession electron diffraction and electron crystallography Chairs: S. Nicolopoulos, J. Gjønnes	Decision making and algorithms for automation in macromolecular structure solution Chairs: H. Powell, R. Hoofft
MS.39.1(C72) T. Proffen: Total scattering: The key to the local and medium range structure of complex materials	MS.40.1(C74) J. S. Loveday: High pressure studies of planetary ices	MS.41.1(C75) C. J. Gilmore: Solving zeolite structures using electron crystallography	MS.42.1(C77) N. Kunishima: High-throughput crystallization-to-structure pipeline at RIKEN SPring-8 Center
MS.39.2(C72) T. Otomo: New opportunity to explore noncrystalline materials by neutron total diffractometer (NOVA) at J-PARC	MS.40.2(C74) H. Fukazawa: Nucleation and growth of ice XI -Study suggests the existence of ferroelectric ice in the Universe-	MS.41.2(C75) J. P. Abrahams: Prospects for structure solution by electron diffraction of three-dimensional protein crystals	MS.42.2(C77) J. M. Holton: There and back again: Using simulated diffraction images to optimize data processing by Elves
MS.39.3(C73) D. A. Keen: Negative thermal expansion and local crystal structure	MS.40.3(C74) K. Hirose: High-pressure phase transitions of deep Earth materials	MS.41.3(C76) J-P. Morniroli: Symmetry determinations from electron precession: Comparison and advantages with CBED	MS.42.3(C77) B-C. Wang: Signal-based data collection: A novel approach to on-site auto-structure determination at SER-CAT
MS.39.4(C73) V. Petkov: High-resolution structure of disordered materials by high-energy X-ray diffraction	MS.40.4(C75) M. Avdeev: Perovskites ABX ₃ under pressure: Transition to post-perovskite CaIrO ₃ type and other scenarios	MS.41.4(C76) S. Hovmöller: Quantitative 3D electron diffraction data by precession and electron rotation methods	MS.42.4(C78) S. Panjekar: Auto-Rickshaw: An online tool for validation of an X-ray diffraction experiment
MS.39.5(C73) S. Shamoto: Atomic pair distribution function analysis on nanomaterials	MS.40.5(C75) P. H.J. Mercier: <i>Ab-initio</i> crystallography of kaolin minerals: Synthesis, diagenesis and mantle pressures	MS.41.5(C76) W. Sinkler: Models for simplified treatment of precession electron diffraction	MS.42.5(C78) C. Vonrhein: AutoPROC - A framework for automated data processing