Memo

Afternoon Session 16:30-17:30

A-05MH *(PL 2)*

PL02*(C2)* | **Kurt Wüthrich**:
NMR in solution and X-ray diffraction in crystals for postgenomic biology

Chair: **Eddy Arnold**

Morning Session 8:30-9:30

A-05MH *(KN 34)*

KN34*(C12)* | **Andrzej Joachimiak**:
Focused structural genomics

Chair: **Liang Tong**

F-12CH *(KN 35)*

KN35*(C12)* | **Jochen R. Schneider**:
Science at XUV and hard X-ray free electron lasers

Chair: **Akira Kira**

D-1003 *(KN 36)*

KN36*(C13)* | **Roberta Oberti**:
Structure refinement and structure modelling: A chemical probe for complex mineral groups

Chair: **Wulf Depmeier**

Time	A-05MH **(MS 85)**	F-12CH **(MS 86)**	D-1003 **(MS 87)**
9:55–10:00 Opening Remarks	**Structural proteomics, focused structural proteomics** Chairs: **M. Tanokura, R. Page**	**Perovskites and related materials** Chairs: **D. Pandey, C. J. Howard**	**Design and applications of nanoscale materials** Chairs: **S. Takamizawa, J. J. Vittal**
10:00–10:30	**MS.85.1**(C143) **J. Weigelt**: Structural genomic of protein families and pathways in human disease	**MS.86.1**(C144) **P. M. Woodward**: Complex perovskites: Chemical order, crystallographic distortions and physical properties	**MS.87.1**(C146) **M. Kawano**: Crystallographic direct observation of chemical reactions in a pore
10:30–11:00	**MS.85.2**(C143) **I. A. Wilson**: Structural genomics and the expanding protein universe	**MS.86.2**(C144) **M. Catti**: Local and long-range structure in LLTO perovskites with Li^+ superionic mobility	**MS.87.2**(C146) **P. Thiyagarajan**: Phase behavior of block copolymer/ inorganic nanocomposites
11:00–11:30	**MS.85.3**(C143) **R. Page**: Using focused structural proteomics to elucidate the molecular basis of MAPK regulation in T cells	**MS.86.3**(C144) **J-M. Kiat**: Size and strain effects in nanostructured relaxor and morphotropic compounds	**MS.87.3**(C146) **K. P. Loh**: From molecular clusters to nanocrystals - Optical and magnetic properties of metal sulfides
11:30–12:00	**MS.85.4**	**MS.86.4**(C145) **Y. Kuroiwa**: Thermal motion of atoms in cubic structure of perovskites and ferroelectric phase transitions	**MS.87.4**(C147) **R. Theissmann**: *In-situ* transmission electron microscopy and theoretical studies on the coalescence of nanoparticles
12:00–12:30	**MS.85.5**(C144) **S. Yokoyama**: Focused structural proteomics of protein synthesis systems	**MS.86.5**(C145) **R. Schierholz**: The system of $PbZr_{1-x}Ti_xO_3$ studied by convergent-beam electron diffraction (15 min)	**MS.87.5**(C147) **J. Bak-Misiuk**: Structural and magnetic properties of MBE grown MnSb layers
		MS.86.6(C145) **J. Bezjak**: The synthesis, crystal structural study and microwave dielectric properties of $Ba_6WNb_2O_{14}$ (15 min)	

C-1001, 2 **(MS 88)**	G-1202 **(MS 89)**	B-05SH **(MS 90)**	E-1009 **(MS 91)**
Algorithmic developments for solving and refining periodic and aperiodic structures Chairs: **H. Fan, M. Lutz**	**Space groups and their generalizations: A tribute to E. Ascher and J.J. Burckhardt** Chairs: **H. Grimmer, M. Nespolo**	**New X-ray sources: ERLs, table top SR, (X)FELs** Chairs: **G. Materlik, T. Matsushita**	**Spinel - geometrically frustrated system: Dedicated to Prof. Nishikawa** Chairs: **K. Kakurai, B. Chakoumakos**
MS.88.1(C147) **M. Merli**: Leverage analysis: A statistical tool to enhance the control on the crystal structure refinement	**MS.89.1**(C149) **A. Janner**: Experiencing space groups	**MS.90.1**(C150) **L. N. Johnson**: Life sciences at Diamond Light Source and prospects with new light sources	**MS.91.1**(C152) **H. Takagi**: Liquid state of spins and charges in geometrically frustrated spinel oxides
MS.88.2(C148) **H. Puschmann**: Small-molecule refinement using the computational crystallography toolbox (cctbx) with Olex2	**MS.89.2**(C149) **I. Orlov**: Space groups resulting from 3D sections of (3+1)D superspace groups. Can all 3D groups be generated?	**MS.90.2**(C151) **T. Ishikawa**: A compact X-ray free electron laser at SPring-8	**MS.91.2**(C152) **D. Louca**: Local order and frustration in vanadate spinels
MS.88.3(C148) **A. O. Madsen**: Anisotropic displacement parameters for molecular crystals from periodic HF and DFT calculations	**MS.89.3**(C149) **P. Zeiner**: Space groups, subgroups and a lot more	**MS.90.3**(C151) **S. M. Gruner**: Status of the Energy Recovery Linac (ERL) project at Cornell University	**MS.91.3**(C152) **A. S. Wills**: Controlling spin glass entropy - Frustrated magnetism in the spinels
MS.88.4(C148) **M. Dusek**: Joint refinement of single crystal and powder data from X-ray and neutron sources	**MS.89.4**(C150) **B. Souvignier**: J.J. Burckhardt's contributions to crystallography	**MS.90.4**(C151) **H. Yamada**: Electron storage ring based tabletop light source named MIRRORCLE for protein crystallography	**MS.91.4**(C153) **N. Ishizawa**: Polaronic behavior of Mn_4O_4 heterocubane clusters in $LiMn_2O_4$ spinel
MS.88.5(C149) **R. De Gelder**: FIDDLE: A method for simultaneous indexing and structure solution from powder diffraction data	**MS.89.5**(C150) **Y. Teshima**: Heterogeneous cylinder packing: Space group on periodic structures with <110> six directions	**MS.90.5**(C152) **W. S. Graves**: Integrating laser and linac technology for next generation X-ray sources	**MS.91.5**(C153) **O. Pieper**: Magnetic structure of the quasi-one-dimensional, frustrated, spin-1 antiferromagnet CaV_2O_4

Saturday, August 30 - Afternoon - **Microsymposia**

Time	A-05MH **(MS 92)**	F-12CH **(MS 93)**	D-1003 **(MS 94)**
13:45–13:50 Opening Remarks	**Structural informatics and database** Chairs: **Z. Dauter, J. Richardson**	**RNA and DNA structures** Chairs: **A. Takenaka, A. Dock-Bregeon**	**Complementary low-Z element absorption spectroscopy by X-ray Raman scattering** Chairs: **U. Bergmann, E. Holub-Krappe**
13:50–14:20	**MS.92.1**(C153) **A. M. Buckle**: Federated repositories of X-ray diffraction images (25 min)	**MS.93.1**(C155) **E. Westhof**: The annotations of non-Watson-Crick base pairs and comparisons between RNA structures and sequences	**MS.94.1**(C157) **C. Sternemann**: X-ray Raman scattering: A probe of soft X-ray absorption edges using hard X-rays
14:20–14:50	**MS.92.2**(C154) **J. E. Johnson**: Virus particle explorer: An X-ray and electron microscopy database for icosahedral virus structures (25 min)	**MS.93.2**(C156) **Y-I. Chi**: Capturing hammerhead ribozyme structures in action by modulating the rate of general base catalysis	**MS.94.2**(C157) **S. K. Lee**: Pressure-induced structural transition in oxides at high pressure: Inelastic X-ray scattering study
14:50–15:20	**MS.92.3**(C154) **W. Minor**: Metal and small molecule agent environment in macromolecules (25 min)	**MS.93.3**(C156) **G. N. Parkinson**: Ligand binding and structural rearrangements of quadruplexes containing human telomeric sequences	**MS.94.3**(C157) **S. T. Gerald**: New applications of q-dependent XRS across the periodic table
15:20–15:50	**MS.92.4**(C154) **M. S. Weiss**: On atomic displacement parameters and coordinates in protein structures (25 min)	**MS.93.4**(C156) **M. M. Georgiadis**: Crystal structures of DNA-bound Co(III)·bleomycins	**MS.94.4**(C158) **J. S. Tse**: X-ray Raman of water in the condensed phases
15:50–16:20	**MS.92.5**(C155) **T. Lutteke**: Quality checks for carbohydrate structures in PDB entries (25 min)	**MS.93.5**(C156) **C. J. Cardin**: Molecular recognition and the DNA Holliday junction	**MS.94.5**(C158) **Y. Cai**: High-resolution X-ray Raman scattering and the study of ices under high pressure
	MS.92.6(C155) **J. Westbrook**: Data quality in the PDB archive (30 min)		

C-1001, 2 **(MS 95)**	G-1202 **(MS 96)**	B-05SH **(MS 97)**	E-1009 **(MS 98)**
Microanalysis of cultural heritage Chairs: **Y. Terada, W. Kockelmann**	**Programming for CIF and related file structures** Chairs: **I. David Brown, I. Guzei**	**New X-ray detectors : Pixel detectors** Chairs: **M. Tate, P. Fajardo**	**Knowledge-based applications in structural chemistry** Chairs: **M. Winn, J. van de Streek**
MS.95.1(C158) **P. Paufler**: Nanostructure of ancient Damascus blades	**MS.96.1**(C159) **N. Spadaccini**: CIF and a new DDL − What it can do; How it is done	**MS.97.1**(C161) **K. Hattori**: Performance of micro pixel gas chamber in small angle X-ray scattering experiments	**MS.98.1**(C163) **R. Subramanian**: Quality of protein crystal structures in the protein data bank
MS.95.2(C158) **K. O. Yamahana**: Scientific contribution to archaeology: Fingerprinting the ancient Egyptian objects	**MS.96.2**(C160) **J. R. Hester**: CIF software in a DDLm world	**MS.97.2**(C161) **R. D. Durst**: High speed readout of microgap X-ray detectors	**MS.98.2**(C163) **J. M. Cole**: Discovering the world's best organic non-linear optical materials
MS.95.3(C159) **E. Kotulanova**: Salt corrosion of lead-based pigments: Laboratory experiments and analysis of ancient frescoes	**MS.96.3**(C160) **H. J. Bernstein**: Transition to object-oriented data representations: Interconversion between CIF and other formats	**MS.97.3**(C162) **C. Broennimann**: The PILATUS detectors: Hybrid pixel detectors for synchrotron and industrial applications	**MS.98.3**(C163) **S. Huth**: The crystal structures of para-acetanilides analysed systematically
MS.95.4	**MS.96.4**(C160) **M. I. Aroyo**: The bilbao crystallographic server	**MS.97.4**(C162) **G. A. Carini**: Monolithic active-matrix silicon X-ray detectors	**MS.98.4**(C163) **S. J. Fisher**: An investigation into deuteration effects: Implications for protein crystallography
MS.95.5(C159) **E. Dooryhée**: Structural investigations of archaeological hybrid materials	**MS.96.5**(C161) **B. McMahon**: publCIF: A complete crystal structure publishing environment for authors	**MS.97.5**(C162) **A. S. Schwarz**: The 2D X-ray detector development program for the European XFEL	**MS.98.5**(C164) **T. N. Bhat**: Structural database using semantic Web concepts to support structure-Based drug design for AIDS