American Crystallographic Association
New Orleans 2011

# ANNUAL MEETING

## May 28 - June 2, 2011
## New Orleans, LA

# *Program*

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# American Crystallographic Association
# 2011 Annual Meeting
# May 28 - June 2
# New Orleans, LA

Program Chair: Chris Cahill
Local Committee: Cheryl Stevens, Ed Stevens, Frank Fronczek
Poster Chair: Ilia Guzei

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# www.AmerCrystalAssn.org

## About the ACA

The American Crystallographic Association (ACA) was founded in 1949 through a merger of the American Society for X-Ray and Electron Diffraction (ASXRED) and the Crystallographic Society of America (CSA). The objective of the ACA is to promote interactions among scientists who study the structure of matter at atomic (or near atomic) resolution. These interactions will advance experimental and computational aspects of crystallography and diffraction. They will also promote the study of the arrangements of atoms and molecules in matter and the nature of the forces that both control and result from them.

Membership in the ACA is open to any person who is actively interested in the purposes of the Association and whose application is approved by the ACA Council or its designee. All members are entitled to voting privileges. Student members are very welcome and their contributions to the life and vigor of the association has always been important. The benefits of membership are the same in all categories. These include: voting privileges, RefleXions, the ACA newsletter that is published 4 times per year, complimentary subscription to the Newsletter of the International Union of Crystallography, and Physics Today, a monthly publication of AIP, and reduced rates for the International Tables for X-Ray Crystallography, Structure Reports, Journal of Applied Crystallography, and Acta Crystallographica when purchased for the member's personal use only. The ACA is a member society of the American Institute of Physics (AIP) and an Affiliate Member of the International Union of Crystallography.

The total membership of the ACA is about 2,200. National meetings are held annually. There are 12 Special Interest Groups (SIG's) concerned with Biological Macromolecules, Fiber Diffraction, General Interest, Industrial, Materials Science, Neutron Scattering, Powder Diffraction, Service Crystallography, Small Angle Scattering, Small Molecules, Synchrotron Radiation and Young Scientists. Members may join as many of these groups that are of interest them. Each Special Interest Group is responsible for organizing sessions at Annual Meetings at least every other year.

The headquarters of the association is located at Hauptman Woodward Medical Research Institute, 700 Ellicott St., Buffalo, NY 14203.

# SATURDAY, MAY 28

## WK.01 Symmetry-mode Analysis

Chair: Branton Campbell
Maurepas

**08:00-08:30am Introduction to symmetry-mode analysis (M. Perez-Mato)**

- Distortions and their order parameters (strain, displacive, occupational, magnetic).
- Symmetry modes are a relative description that depends on the parent structure.
- Irreps of the parent symmetry and their basis functions.
- Irrep basis functions provide a symmetry-motivated basis for distortions.
- Define distortion symmetry and isotropy subgroup (single-irrep distortion).
- Irrep coupling to get more complicated distortions.

**08:30-10:00am Exploring structural distortions with ISODISTORT (B. Campbell and H. Stokes)**

- Distortion output:

Distortion symmetry – specifies space-group type, origin and basis
Visualization tools, CIF, mode details, primary OPs, domains, other

- Filtered search tools for generating distortion models:

Database search – commensurate single-irrep distortions
Search by supercell and space-group type
Search by k-point/irrep/OPD

- Domains
- Primary vs secondary order parameters
- Coupled order-parameters
- Incommensurate example and superspace-symmetry

**10:00-10:30am** Coffee break

**10:30-12:00pm Symmetry mode analysis with AMPLIMODES & FULLPROF (M. Perez-Mato)**

- Define mode amplitudes
- Mode-decomposition examples
- Order-parameter evolution near a phase transition and critical exponents
- Symmetry-mode refinement(s) using Fullprof

**12:00-01:00pm** Lunch break

**01:00-02:30pm Symmetry-mode analysis with ISODISTORT & TOPAS (B. Campbell and H. Stokes)**

- Work through mode decomposition examples
- Work through symmetry-mode refinement(s) using TOPAS
- How to "solve" a distorted structure on the symmetry-mode basis

**02:30-03:00pm Magnetic symmetry (H. Stokes)**

- Review magnetic symmetry and nomenclature
- Walk users through the online magnetic-symmetry database
- The relationship between the OG and BNS settings
- How to describe a magnetic structure
- The relationship between the OG and BNS settings

**03:00-03:30pm** Coffee break

**03:30-04:30pm Magnetic distortions (M. Perez Mato)**

- Introduce magnetic distortions
- Examples using ISODISTORT
- An incommensurate magnetic distortion

**04:30-05:00pm Magnetic symmetry-mode refinement (B. Campbell)**

- A magnetic refinement using TOPAS
- Many magnetic structures are "solved" now in P1. Emphasize utility of mag symmetry

## WK.02 Introduction to PHENIX for Beginning to Advanced Crystallographers

Chair: Paul Adams
Borgne

**08:30am** PHENIX Overview (Paul Adams)

**08:50am** Automation of Structure Determination in PHENIX (Tom Terwilliger)

**09:35am** Break and set-up of PHENIX on individual computers

**10:00am** Molecular Replacement (Paul Adams)

**10:45am** Refinement with X-rays and neutrons in PHENIX (Pavel Afonine)

**11:30am** Structure Validation (Chris Williams)

**12:15pm** Lunch break

**01:00 - 02:00pm** Group Tutorial -- Data analysis and Structure solution

**02:00 - 03:00pm** Group Tutorial -- Model-building and Ligand Fitting

**03:00 - 03:30pm** Coffee break

**03:30 - 04:3pm** Group Tutorial -- PHENIX Refinement and Validation

### New Student Orientation

**06:30pm D1**
**Chair: Eric Armstrong**

The focus of this informal session is to orient 'young scientists' and first time attendees to the structure of the ACA Meeting and how to make the most of their experience.

### Opening Reception Exhibit Show and Presidential Welcome

07:30pm Napoleon Ballroom

# SUNDAY, MAY 29

| | | |
|---|---|---|
| Registration Desk | 07:30am | Napoleon Foyer |
| Speaker Ready Room | 07:30am | Oakley, 4th floor |
| Council Meeting Room | 07:30am | Nottoway, 4th floor |
| Exhibit Show | 10:00am | Napoleon Ballroom |

## SP.01 2011 Margaret C. Etter Early Career Award

**Chair: Jamaine Davis**
**D2-D3**
**Award presentation to Yurij Mozharivskyj by President Thomas Koetzle .**

**08:00am-08:50am** **SP.01.1**
Chemistry of Re5X4 Magnetocaloric Phases: Interplay Between Electron Concentration and Crystal Structure. Yurij Mozharivskyj.

## SP.01 Etter Early Career Award Symposium

Chair: Jamaine Davis
D2-D3

**09:00-09:20am** **SP.01.2**
Spy: a New Class of Molecular Chaperones. Karen Ruane, Shu Quan, James C.A. Bardwell, Rong Shi, Miroslaw Cygler.

**09:20-09:40am** **SP.01.3**
Insights Into Structure-Function Relationships in GTPase-Effector Interaction. Badri Nath Dubey, Lothar Gremer Gremer, Radovan Dvorsky, Mohammad Reza Ahmadian.

**09:40-10:00am** **SP.01.4**
Detergent, Bicelle, and LCP Crystallization of the Outer Membrane Protein Intimin from Enterohemorrhagic *E. coli* (EHEC). James Fairman, Travis Barnard, Nicholas Noinaj, Susan Buchanan.

**10:00-10:30am** Coffee break

**10:30-10:50am** **SP.01.5**
Structural Insights Into the Role of Protein Surface Flexibility in the Regulation of Polo-Like Kinase 1. Pawel Sledz, Steffen Lang, Christopher Stubbs, Grahame McKenzie, Ashok Venkitaraman, Marko Hyvonen, Chris Abell

**10:50-11:05am** **SP.01.6**
Structural Mechanism for Activation of the Orphan Nuclear Receptor Lrh-1 by Small Molecule and Lipid Agonists. Paul Musille, Eric Ortlund.

**11:05-11:20am** **SP.01.7**
Structure of the Human RON Receptor Tyrosine Kinase in Complex With the MSP β-Chain. Kinlin Chao, I-Wei Tsai, Natalia Gorlatova, Chen Chen, Osnat Herzberg.

**11:20-11:40am** **SP.01.8**
Crystal Structure of a Clade C HIV-1 gp120 Bound to Cd4 and Cd4-Induced Antibody. Ron Diskin, Paola Marcovecchio, Pamela Bjorkman.

**11:40-12:00pm** **SP.01.9**
Crystal Structure of Human Dual-Specificity Phosphatase 27, An Atypical DUSP. George Lountos, Joseph Tropea, David Waugh.

| | | |
|---|---|---|
| Canadian Div. Meeting | 12:00pm | D1 |
| General Interest Group Meeting | 12:00pm | Maurepas |
| Poster Session P-S | 05:30pm | Napoleon Ballroom |
| Rayonix Young Scientist Mixer (ticket required) | 08:00pm | Waterbury Ballroom, 2nd floor |

## 01.01 Use of Databases in Structural Biology

Chair: Wladek Minor
Borgne

**09:00-09:30am** **01.01.1**
Putting the "Data" in "Data Mining": Curating the PDB Archive. Helen Berman, Gerard Kleywegt, Haruki Nakamura, John Markley.

**09:30-10:00am** **01.01.2**
Biomolecular Interactions: a New Look at NCBI's Structural Biology Information Resources. Stephen Bryant.

**10:00-10:30am** Coffee break

**10:30-11:00am** **01.01.3**
Virus Particle Explorer: An X-Ray and Electron Microscopy Database for Icosahedral Virus Structures. John Johnson.

**11:00-11:30am** **01.01.4**
Protein Structural Similarity: Tools, Databases, and Problems. Adam Godzik.

**11:30-11:50am** **01.01.5**
Databases Promote Efficiency at NSLS/PXRR MX Beamlines. Howard Robinson, Rick Buono, Matt Cowan, John Skinner, Bob Sweet, Annie Heroux.

**11:50-12:00pm** **01.01.6**
Using Small Molecule Crystal Structure Data for Ligands in Protein-Complex Structure Determination. Thomas Womack, Gerard Bricogne, Claus Flensburg, Peter Keller, Wlodek Paciorek, Andrew Sharff, Clemens Vonrhein, Oliver Smart.

**12:10-12:30pm** **01.01.7**
Enhancements to the LabDB Crystallographic Laboratory Information Management System. Matthew Zimmerman, Kamila Wojciechowska, Wojtek Wajerowicz, Zbigniew Fratczak, Wladek Minor.

## 02.01 General Interest I

Chair: Peter Mueller
Maurepas

**09:00-09:15am** **02.01.1**
Crystal Growth of Monosodium Urate Monohydrate. Jennifer Swift, Clare Perrin.

**09:15-09:30am** **02.01.2**
Resolution of Racemic Pharmaceuticals Via Crystallization on Chiral Templates. John MacDonald, Pranoti Navare.

**09:30-09:45am** **02.01.3**
Massively Parallel Geometric Computations of Small Molecule Crystal Structures. Jason I. Mercer, Louise N. Dawe.

**09:45-10:00am** **02.01.4**
New Models in Mathematical Crystallography. Olga Smirnova.

**10:00-10:30am** Coffee Break

**10:30-11:00am** **02.01.5**
Lee-Richards Surfaces, Gaussians and Nearest Neighbors. Herbert J. Bernstein, Lawrence C. Andrews.

**11:00-11:30am** **02.01.6**
Crystal Structure Thermal Ellipsoid Dynamics: a Research Prospectus. Carroll Johnson, Michael Burnett, Bryan Chakoumakos.

**11:30-12:00pm** **02.01.7**
Partial Observations, Partial Models and Partial Residuals in Least Squares Refinement. A. David Rae.

# SUNDAY, MAY 29

## 08.01 *In situ* Diffraction Studies

Chairs: Christine Beavers, Craig Bridges
D1

**09:00-09:25** **08.01.2**
Reactivities of Metastable Oxides by *in-situ* Diffraction. Mario Bieringer, Shahid Shafi, Bradley Hernden, Miguel Alario-Franco.

**09:25-09:45am** **08.01.3**
Structural and Magnetic Properties of Cobalt Oxide Under Pressure. Antonio dos Santos, Jamie Molaison, Christopher Tulk, Yansun Yao, Dennis Klug.

**09:45-10:00am** **08.01.4**
Expanding the Power of High Resolution Powder Diffraction; *in-situ* Studies at 11-Bm. Matthew Suchomel, Lynn RibaudArgonne National Laboratory, Haiyan Zhao, Mathieu Allix.

**10:00-10:30am** Coffee Break

**10:30-10:55am** **08.01.5**
Light and Pressure Induced Solid-State Transformations in Dithienylethenes and Their Metal Complexes. Paul Raithby, Simon Brayshaw, Christopher Woodall, Stefanie Schiffers, Anna Stevenson, Mark Warren, David Allan, John Warren, Julia Weinstein.

**10:55-11:10am** **08.01.6**
Thermally-Induced Solid-State Reactions and Phase Transitions: Puzzles and Solutions. Bruce Foxman, C.-H. Chen, Aaron R. Gell, Shai R. Posner.

**11:10-11:35am** **08.01.7**
Temperature Dependent Structural Heterogeneity in Liquids. John Parise, Christopher Benmore, Richard Weber, Lawrie Skinner, Jincheng Du, Lena Lazareva, Martin Wilding.

**11:35-11:50am** **08.01.8**
Controlling Thermal Expansion in a Series of Metal-Organic Framework Materials. Yue Wu, Cameron Kepert.

**11:50-12:00pm** **08.01.9**
*In situ* X-Ray Diffraction Studies of Functional Molecular Materials. Gregory Halder, Karena Chapman, Peter Chupas, John Schlueter, Jamie Manson.

## 04.01 Surfaces and Interfaces

Chair: Zhang Jiang & Masafumi Fukuto
Maurepas

**01:30-02:00pm** **04.01.1**
Soft X-Ray Scattering of Soft Material Thin Films. Cheng Wang, Anthony Young, Howard Padmore, Alexander Hexemer.

**02:00-02:20pm** **04.01.2**
Screening Effect of Highly Compressible Supercritical Carbon Dioxide on Attractive Polymer/Substrate Interactions. Tad Koga, Peter Gin, Naisheng Jiang, Maya Endoh, Bulent Akgun, Sushil Satija.

**02:20-02:40pm** **04.01.3**
Grazing Incidence Small-Angle X-Ray Scattering and X-Ray Spectroscopy *in-situ* Characterization of Nanocatalysts. Randall Winans, Sungsik Lee, Byeongdu Lee, Soenke Seifert, Stefan Vajda.

**02:40-03:00pm** **04.01.4**
Strain-Field Measurement of Iron Silicides Thin Films Using X-Ray Bragg-Surface Diffraction. Chia-Hung Chu, Yi-Wei Tsai, Mau-Tsu Tang, Shih-Lin Chang.

**03:00-03:30pm** Coffee Break

**03:30-04:00pm** **04.01.5**
Surfaces Sensitive and Ion-Specific X-Ray Spectroscopy and Diffraction at Liquid Interfaces. David Vaknin.

**04:00-04:30pm** **04.01.6**
Structure and Interactions in Two-Dimensional Assemblies of Tobacco Mosaic Viruses on a Substrate-Supported Lipid Monolayer. Lin Yang, Suntao Wang, Masafumi Fukuto, Zhongwei Niu, Qian Wang.

**04:30-05:00pm** **04.01.7**
The Effect of Aqueous Chemistry on Nucleation and Growth of Iron Oxide Nanoparticles at Environmentally Relevant Interfaces. Young-Shin Jun, Glenn Waychunas, Byeongdu Lee, Jessica Ray, Yandi Hu.

## 08.02 Structural Enzymology I: Spectroscopy and Complementary Methods

Chair: Allen Orville
Borgne

**01:30-02:00pm** **08.02.1**
Quaternary Ammonium Oxidative Demethylation: X-Ray Crystallographic and On-Beam Raman and UV-Visible Spectroscopic Characterization of a Rieske-Type Demethylase. Karen Allen, Kelly Daughtry, Youli Xiao, Deborah Stoner-Ma, Allen Orville, Pinghua Liu.

**02:00-02:30pm** **08.02.2**
This Side Or the Other? Selective Cleavage at the S-Adenosylmethionine Sulfur Atom by a Radical [4Fe-4S]-Containing Enzyme. Andrew Torelli, Yang Zhang, Xuling Zhu, Hening Lin, Steven E. Ealick.

**02:30-03:00pm** **08.02.3**
Single Crystal XAS Studies on Metalloprotein Intermediates. Ritimukta Sarangi, Britt Hedman.

**03:00-03:30pm** Coffee Break

**03:30-04:00pm** **08.02.4**
Insights Into the Mechanism of Heme Degradation by the Isdg-Like Family of Enzymes. Michael Murphy, Georgia Ukpabi, Sarah Thackray.

**04:00-04:30pm** **08.02.5**
Crystal Structures of the CO and NO Adducts of MauG in Complex With Pre-Methylamine Dehydrogenase: Implications for the Mechanism of Oxygen Activation. Erik Yukl, Brandon Goblirsch, Victor Davidson, Carrie Wilmot.

**04:30-05:00pm** **08.02.6**
Defining the Role of the Axial Ligand of the Type 1 Copper Site in Amicyanin, An Electron Transfer Protein from *Paracoccus denitrificans*. Narayanasami Sukumar, Moonsung Choi, Victor Davidson.

## 08.03 Crystallography and the Search for New Materials

Chair: Svilen Bobev
D1
*sponsored, in part, by Agilent Technologies, Bruker AXS, Inc., and Rigaku Americas Corp.*

**01:30-01:55pm** **08.03.1**
Insights Into Solid-State Oxide and Intermetallic Structure-Property Relations From Diffraction Experiments. Robin Macaluso, Han-yul Hong, Theeranon Siritanon, Geneva Plankis, Arthur Sleight, Mas Subramanian.

**01:55-02:15pm** **08.03.4**
Ferecrystals. Matt Beekman, Mary Smeller, Paul Zschack, Michael Anderson, Ian Anderson, Ryan Atkins, Krista Hill, Dan Moore, Ngoc Nguyen, David Johnson.

**02:15-02:35pm** **08.03.6**
Single Crystal Growth and Structure Determination of Complex Metal Hydroxides. Daniel Bugaris, William Chance, Hans-Conrad zur Loye.

**02:35-03:00pm** **08.03.8**
Chemical Frustration: Lessons on Materials Design From Complex Intermetallics. Daniel Fredrickson, Veronica Berns, Rie Fredrickson, Amelia Hadler, Nicholas Harris, Michael Sapiro, Patrick Sims, Timothy Stacey.

**03:00-03:30pm** Coffee Break

**03:30-03:55pm** **08.03.9**
Mixed Crystal Formation and Structural Studies in the Mullite-Type System Bi2Fe4O9-Bi2Mn4O10. Michael Lufaso, Zachary Kann, Jeffrey Auletta, Eric Hearn, Sven-U. Weber, Klaus Weber, Hartmut Schneider.

**03:55-04:15pm** **08.03.11**
The Challenge of Aluminum Monophenyl Diphosphonate. Tiffany Kinnibrugh, Nancy Garcia, Bram Carlson, Abraham Clearfield.

**04:15-04:35pm** **08.03.12**
Synthesis & Structure of Gd(Mn, Al)12 and GdMn2Al10. Bradford Fulfer, Julia Chan.

**04:35-05:00pm** **08.03.13**
Conventional and Unconventional Crystallographic Investigations Into Materials for Photocatalysis and Other Energy Applications. Peter Khalifah.

## 08.04 Scholarly and Pragmatic Aspects of Crystallographic Publication Practices

Chairs: Larry Falvello & Ilia Guzei
D2-D3
*sponsored, in part, by Agilent Technologies, Bruker AXS, Inc., and International Union of Crystallography*

**01:30-01:55pm** **08.04.1**
Crystallographic Publication in IUCr Journals: Simplifying the Publishing Process. Michael Hoyland.

**01:55-02:15pm** **08.04.2**
Crystallographic Publication Toolbox in an Undergraduate Environment. Jerry Jasinski.

**02:15-02:40pm** **08.04.3**
CheckCIF and CIF in a Multi-User Crystallography Facility. Richard Cooper.

**02:40-03:00pm** **08.04.4**
Structure Validation and Manuscript Preparation with Apex2. Bruce C. Noll, Charles F. Campana, Kaercher Joerg.

**03:00-03:30pm** Coffee Break

**03:30-03:50pm** **08.04.5**
From Independence to Service and Science to Technology: An Evolutionary Tale. Judith Flippen-Anderson.

**03:50-04:15pm** **08.04.6**
Crystallographic Publication in the American Chemical Society Journal Crystal Growth & Design: An Editor's Perspective (So Pay Attention!). Robin Rogers.

**04:15-04:40pm** **08.04.7**
What's Acceptable and What's Not: An Attempt to Find Standards for Chemically Important Structures. Arnold Rheingold, Curtis Moore.

**04:40-05:00pm**
Open Discussion Session. Ilia Guzei, Larry Falvello.

| | | |
|---|---|---|
| Registration Desk | 07:30am | Napoleon Foyer |
| Speaker Ready Room | 07:30am | Oakley, 4th floor |
| Council Meeting Room | 07:30am | Nottoway, 4th floor |
| Exhibit Show | 10:00am | Napoleon Ballroom |
| Agilent Technologies X-ray Cr Workshop (invitations available at the Agilent Technologies booth #107) | 12:00pm | Grand Chenier, 5thFloor |
| Bruker AXS Luncheon | 12:00pm | off site (by invitation only) |
| Synchrotron Radiation SIG Meeting | 12:00pm | D2-D3 |
| BioMac SIG Meeting | 05:00pm | Borgne |
| Poster Session P-M | 05:30pm | Napoleon Ballrooom |
| Fiber Diffraction SIG Gathering | 06:00pm | ACA Registration Desk |
| Mentor/Mentee Dinner (ticket required) | 08:00pm | off site |

## SP.02 Plenary Lecture:
**Philip Coppens, University of Buffalo**
**D2-D3**

**08:00-08:50am** **SP.02.1**
From the Sun to Femtosecond Lasers and Back: Photo-Induced Dynamic Processes in Solids.

## 01.02 Protein Structure Initiative: Tools for the Home Lab
Chair: Ward Smith
Borgne

**09:00-09:20am** **01.02.1**
High-Throughput Crystallization Screening for the Structural Biology Community. Michael Malkowski, Eleanor Cook, Mary Koszelak-Rosenblum, Angela Lauricella, Raymond Nagel, Elizabeth Snell, Jennifer Wolfley, Edward Snell, Joseph Luft, George DeTitta.

**09:20-09:40am** **01.02.2**
ACMI: Towards Automatic Crystallographic Map Interpretation at Low Resolution. George Phillips, Ameet Soni, Craig Bingman, SIddharth Puthur, Jude Shavlik.

**09:40-10:00am** **01.02.3**
Cell-Free Translation in Membrane Protein Research. Brian Fox, David Aceti, Khaled Aly, James Bangs, Emily Beebe, Craig Bingman, Uyen Chu, Darius Chow, Michael Goren, Lianwang GuoKatarzyna Gromek, Katrina Forest, Ronnie Frederick, Shin-ichi Makino, John Markley, Karl Nichols, George Phillips, John Primm, Arnold Ruoho, Donna Troestler, Russell Wrobel, Zsolt Zolnai.

**10:00-10:30am** Coffee Break

**10:30-10:50am** **01.02.4**
Structural Proteomics of Eukaryotic Membrane Proteins. Robert Stroud, John Pak, William Harries, Avner Schlessinger, Louis Metzger, Andrew Waight, Bjorn Panyella Pedersen, Zygy Roe-Zurz, Sarika Chaudhary, Larry Miercke, Joseph D. O'Connell III, Yaneth Robles, Rebecca Robbins, Meseret Tessema, James Holton, Andrej Sali.

**10:50-11:10am** **01.02.5**
The Structural Biology Knowledgebase - a Portal to Protein Sequences, Structures, Functions, Methods and More. Margaret Gabanyi, John Westbrook, Wendy Yi-Ping Tao, Raship Shah, David Micallef, William McLaughlin, Torsten Schwede, Paul Adams, Wladek Minor, Helen Berman.

**11:10-11:30am** **01.02.6**
Using the PSI: Biology-Materials Repository: a Biologist's Resource for Protein Expression Plasmids. Catherine Cormier, Jin Park, Michael Fiacco, Jason Steel, Jason Kramer, Preston Hunter, Rajeev Singla, Joshua LaBaer.

## 04.02 Small Angle Scattering From Colloids

Chair: Gregory Beaucage & P. Russo
D1

**09:05-09:30am** **04.02.1**
Structural Changes in BP Crude Oil During Degradation. Henning Lichtenberg, Amitava Roy, Edward Overton.

**09:30-09:55am** **04.02.2**
Capillary Interactions in Nano-Particles Suspensions. Dobrin Bossev.

**10:00-10:30am** Coffee break

**10:30-10:55am** **04.02.3**
Phase Reorganisation in Self-Assembled Systems Through Interparticle Material Transfer. Christian Moitzi, Anniina Salonen, Stefan Salentinig, Samuel Guillot, Gerhard Fritz-Popovski, Otto Glatter.

**10:55-11:20am** **04.02.4**
Protein Localization in Silica Nanospheres Derived via Biomimetic Mineralization. Volker Urban, Mateus B. Cardoso, Heather R. Luckarift, Hugh O'Neill, Glenn R. Johnson.

**11:20-11:45am** **04.02.5**
Synthesis, Characterization, and Catalysis of Apoferritin Encapsulated Core-Shell Bimetallic Nanoparticles. Byeongdu Lee, Tao Li, Sungsik Lee, Randall Winans.

**11:45-12:00pm** **04.02.6**
A Study of the Supramolecular Properties of Meso-Tetra(4-Sulfonatophenyl)Porphyrin in Aqueous Solutions. Javoris Hollingsworth, Paul Russo, Allison Richard, Graca Vicente.

## 08.07 Materials for a Sustainable Future

Chairs: Ashfia Huq & Claudia Rawn Maurepas

**09:00-09:30am** **08.07.1**
The Search for Rapid Pathways to Synthesize CuInxGa1-xSe2 Thin Film PV Absorbers. Tim Anderson, Ranga Krishnan, Christopher Muzzillo, Woo Kyoung Kim, Andrew Payzant, Carelyn Campbell, Jianyun Shen.

**09:30-10:00am** **08.07.2**
Phase Transitions in Cu-Sb-Se and Ag-Mg-Sb Thermoelectric Materials. Melanie Kirkham, Antonio Moreira Dos Santos, Claudia Rawn, Jeff W. Sharp, Alan J. Thompson, Paul Majsztrik, Eric Skoug, Donald Morelli, E. Andrew Payzant, Edgar Lara-Curzio.

**10:00-10:30am** Coffee Break

**10:30-11:00am** **08.07.3**
Causes of Ion Selectivity in Porous Silicates. Aaron Celestian, Samantha Kramer, Kristin Leftwich.

**11:00-11:20am** **08.07.4**
Structural Changes of the Type-I Clathrate Ba8AlxSi46-x (X = 8, 10, 12, 14, 16) Revealed by Neutron Powder Diffraction. John Roudebush, Clarina Dela Cruz, Bryan Chakoumakos, Susan Kauzlarich.

**11:20-11:40am** **08.07.5**
Gas Adsorption in Metal-Organic Frameworks With Coordinatively Unsaturated Metals Sites. Wendy L. Queen, Craig M. Brown, Matthew R. Hudson, Kenji Sumida, Eric D. Bloch, Leslie J. Murray, Jeffrey R. Long, David K. Britt, Omar M. Yaghi.

**11:40-12:00pm** **08.07.6**
Visualization of Guest-Host Interactions in Energy Storage Materials Using X-Ray and Neutron Diffraction Methods. Xiaoping Wang, Chi Yang, Mohammad A. Omary, Bryan C. Chakoumakos, Huibo Cao, Abhijit

Pramanick, Christina Hoffmann.

**12:00-01:30am** Lunch Break.

**01:30-02:00pm** **08.07.7**
Crystallography of Flux Pinning Defects in High-Temperature Superconductors. Eliot Specht.

**02:00-02:20pm** **08.07.8**
Insights Into Battery Materials From Pair Distribution Function Methods. Karena Chapman.

**02:20-02:40pm** **08.07.9**
A Small-Angle Neutron Scattering Study of Lithiation in Mesoporous Hard Carbon. Craig Bridges, Xiaoguang Sun, Sheng Dai, Jinkui Zhao.

**02:40-03:00pm** **08.07.10**
*In situ* XRD of Li(Mn15Ni05)O4 Cathodes for Lithium Ion Batteries During Formation and Operation Cycles. Kevin Rhodes, Roberta Meisner, Yoongo Kim, Nancy Dudney, Claus Daniel.

**03:00-03:30pm** Coffee Break

**03:30-04:00pm** **08.07.11**
Sr2Fe1.5Mo0.5O6-δ has Been of Interest as an Anode Material in Solid Oxide Fuel Cells. Hans-Conard zur Loye, Daniel Bugaris, Qiang Liu, Guoliang Xiao, Fanglin Chen.

**04:00-04:20pm** **08.07.12**
Atomic Scale Structure of Anode and Cathode Fine Powder Materials for Li Batteries by Total X-Ray Diffraction. Valeri Petkov.

**04:20-04:40pm** **08.07.13**
Atomic Displacements and Thermal Motion in Triphylite-Lithiophilte, Li(Fe,Mn)Po4, Solid Solution. Bryan C. Chakoumakos, Xiaoping Wang, Huibo Cao.

**04:40-05:00pm** **08.07.14**
Opportunities for in situ Neutron Diffraction Studies of Energy Related Materials. Jason Hodges, Ashfia Huq, Olivier Gourdon, Luke Heroux.

## TR.01 Transactions - Time Resolved and Charge Density in Honor of Philip Coppens

Chair: Yu-Sheng Chen, Peter Lee
D2-D3
*sponsored, in part, by Univ. of Chicago/CARS and Bruker AXS, Inc.*

**09:00-09:10am** Introduction

**09:10-09:40am** **TR.01.1**
X-Ray Transient Absorption Spectroscopy: a Decade and Beyond. Lin Chen.

**09:40-10:10am** **TR.01.2**
Phase Transition Driven by Light: the Key Role of X-Ray Diffraction and Time-Resolved Techniques. Eric Collet, Marylise Buron, Maciej Lorenc, Marina Servol, Roman Bertoni, Ludovic Roudaut, Hiroshi Watanabe, Loic Toupet.

**10:10-10:30am** Coffee Break

**10:30-11:00am** **TR.01.3**
Opto-Magnetic Switchable Character in Fe(II) Spin Crossover Complexes. Yu Wang, Chou-Fu Sheu, Che-Hsiu Shih, Masaki Takata.

**11:00-11:30am** **TR.01.4**
Photo-Crystallographic Studies of Spin-Crossover Molecular Materials. Sebastien Pillet, Dorothea Mader, El-Eulmi Bendeif, Gor Lebedev, William Nicolazzi, Claude Lecomte.

**11:30-12:00pm** **TR.01.5**
X-Ray Lasers for Pump-Probe Studies With a Liquid Jet Injector. John Spence.

**12:00-12:30pm** **TR.01.6**
Time Resolved Laue Crystallography - Moving From 3Rd Generation Sources to Fel Experiments. Marc Messerschmidt.

**12:30-01:30pm** Lunch Break

**Afternoon Chair: Jason Benedict**

**01:30-02:00pm TR.01.7**
Combined Charge Spin and Momentum Densities Refinement: Application to Molecular Magnetic Materials. Claude Lecomte, Maxime Deusch, Nicolas Claiser, Mohamed Souhassou, Sebastien Pillet, Iurii Ciumacov, Beatrice Gillon, Jean Michel Gillet, Dominique Luneau.

**02:00-02:30pm TR.01.8**
Properties of Molecular Materials From Electron Density Distribution. Piero Macchi.

**02:30-03:00pm TR.01.9**
Experimental Essentials for Charge Density Studies. Finn Krebs Larsen, Bo Iversen, Jacob Overgaard, Mette Schmoekel, Mads Ry Joergensen.

**03:00-03:30pm** Coffee break

**03:30-03:55pm TR.01.10**
On Quantitative Structural and Electron Density Studies of Interactions in Molecular Crystals. Krzysztof Wozniak, Anna A. Hoser, Paulina M. Dominiak.

**03:55-04:20pm TR.01.11**
Within and Beyond the Pseudoatom Model. Tibor Koritsanszky.

**04:20-04:40pm TR.01.12**
Characterization of Weak Intra- and Intermolecular Interactions Using Experimental Charge Density Distributions. Edwin Stevens.

**04:40-05:00pm TR.01.14**
Charge Density Studies of Organic-Inorganic [Arbf3]- X+ Compounds - State-of-the-art Techniques in Cutting-Edge Structural Research. Radoslaw Kaminski, Krzysztof Durka, Marek Dabrowski, Janusz Serwatowski, Krzysztof Wozniak.

## 06.01 Undergrad Research Symposium

Chair: Kathereine Kantardjieff
D1

**01:30-02:00pm 06.01.1**
Introduction. Kathereine Kantardjieff.

**02:00-02:30pm 06.01.2**
Single Crystal Growth, Crystallography and Magnetic Properties of Maus' Salt. Mary Parker, Bryan C. Chakoumakos, Huibo Cao.

**02:30-03:00pm 06.01.3**
Steric Effects on the Synthesis of Metal Halide Layers and Clusters. Stephanie Cowin, He Meng, Alicia Beatty.

**03:00-03:30pm** Coffee break

**03:30-04:00pm 06.01.4**
The Expression, Purification, and Crystallization of the H-Nox Regulatory Domain of Bovine Soluble Guanylate Cyclase. Leida Rassouli-Taylor, Elsa Garcin.

**04:00-04:30pm 06.01**
A Model of the Alpha Domain Bound to DNA. Angelica Trammell, Doba Jackson, Chelley Lawson, Samuel Griffin, Ashlee Walters, Tiffany Dean.

## Professional Odysseys

Chair: Jamaine Davis
Rhythms 1 (2nd floor) 1:30pm

**Career Panel**
Lorena S. Beese, James B. Duke Professor of Biochemistry, Duke University

Andy Howe, President and CEO at Emerald BioStructures and BioSystems, Co-Principal Investigator at Seattle Structural Genomics Center for Infectious Disease

Christopher Incarvito, Director, chemical and biophysical instrument center, Yale University

## 08.06 Microcrystals and Back to Merging Datasets

Chairs: Dominika Borek & Alex Soares Borgne

**01:30-02:00pm** **08.06.1**
The Pervasive Problem of Crystal Non-Isomorphism. Zbyszek Otwinowski, Dominika Borek, Johan Hattne, Marcin Cymborowski, Wladek Minor.

**02:00-02:30pm** **08.06.2**
Multi-Crystal Data Reduction at Diamond Light Source. Graeme Winter.

**02:30-03:00pm** **08.06.3**
Multi-Crystal Anomalous Diffraction for Macromolecular Phasing. Qun Liu, Zhen Zhang, Zahra Assur, Filippo Marcia, Wayne Hendrickson.

**03:00-03:30pm** Coffee Break

**03:30-04:00pm** **08.06.4**
Data Collection and Processing From Microcrystals of the Beta2-Adrenergic Receptor. Bill Weis.

**04:00-04:30pm** **08.06.5**
Systematically Study of Frozen Crystals Non-Isomorphism: Example Case of Insulin Crystals. Rita Giordano, Sean McSweeney, Alexander Popov.

**04:30-05:00pm** **08.06.6**
Automated Acoustic Methods for Crystallization, Crystal Improvement, and Crystal Mounting. Alexei Soares, Allen Orville, Krystal Cole, Joseph Olechno, Richard Ellson, John Skinner, Robert Sweet, Annie Heroux, Matthew Engel, Marc Allaire.

## 2011 Margaret C. Etter Student Lecturer Awards

Each Special Interest Group (SIG) has the opportunity to select one student to receive an award and to present a lecture in one of the sessions organized by that SIG. Selections are based upon submitted abstracts and are independent of whether the student originally requested an oral or poster presentation. Award winners are determined by the elected officers of the SIGs. Students who are selected receive a monetary award of $250 and a certificate to be presented at the beginning of their lecture.

**Congratulations to this year's winners:**

BioMac ..... Rebekah Nash, Univ. North Carolina, Chapel Hill ..... 08.09.6
General Interest ..... Jason Mercer, Memorial Univ. of Newfoundland ..... 02.01.3
Materials Science ..... Phoebe Allan, Univ. of St. Andrews, UK ..... 08.08.1
Powder Diffraction ..... Kevin Rhodes, Univ. of Tennessee, Oak Ridge ..... 08.07.10
Small Molecules ..... John Sander, Univ. of Iowa, Iowa City ..... 05.02.13
Small Angle Scattering ..... Thomas Grant, Hauptman-Woodward Inst, Buffalo NY ..... 04.03.5
Synchrotron Radiation ..... Lauren Hatcher, Univ. of Bath, UK ..... TR.01/05.01.4
Young Scientist ..... Karen Ruane, McGill Univ., Montreal Canada ..... SP.01.2

# TUESDAY, MAY 31

| | | |
|---|---|---|
| Registration Desk | 07:30am | Napolean Foyer |
| Speaker Ready Room | 07:30am | Oakley, 4th floor |
| Council Meeting Room | 07:30am | Nottoway, 4th floor |
| Exhibit Show | 10:00am | Napoleon Ballroom l |
| Service & Small Molecules Joint SIG Meeting | 12:00pm | Maurepas |
| Young Scientist SIG Meeting | 12:00pm | D2-D3 |
| ***All Member Business Meeting*** | ***05:00pm*** | ***Maurepas*** |
| Poster Session P-T | 05:30pm | Napoleon Ballroom |

## SP.03 Warren Award to Keith Moffat

**Award presentation to Keith Moffat by President Thomas Koetzle .**
**D2-D3**

**08:00-08:50am** **SP.03.1**
Time-Resolved Macromolecular Crystallography: From Hours to Femtoseconds. Keith Moffat.

## 01.03 Structural Enzymology II - Mechanistic

Chair: Zachary Wood
Borgne

**09:00-09:20am** **01.03.1**
The Structural Basis of Assembly Stimulated GTP Hydrolysis by Human Dynamin. Fred Dyda, Joshua S. Chappie, Sharmistha Acharya, Marilyn Leonard, Sandra L. Schmid.

**09:20-09:40am** **01.03.2**
Characterization of HPXO, a Novel Fad-Dependent Urate Oxidase. Katherine Hicks, Sean O'Leary, Tadhg Begley, Steven Ealick.

**09:40-10:00am** **01.03.3**
Structural Characterization of Human Carbonic Anhydrase II: Modulation of a Catalytically Efficient Enzyme. Dayne West, Jim Gordon, David Silverman, Robert McKenna.

**10:00-10:30am** Coffee Break

**10:30-10:50am** **01.03.4**
The Coupling of Conformational Equilibria and Enzyme Function in Phosphoenolpyruvate Carboxykinase. Todd Holyoak, Troy Johnson, Sarah Holyoak.

**10:50-11:10am** **01.03.5**
Structure of the DNA Glycosylase Alka in Complex With Undamaged DNA. Brian Bowman, Seongmin Lee, Shuyu Wang, Gregory Verdine.

**11:10-11:30am** **01.03.8**
The Crystal Structure of the Intron Debranching Enzyme in Complex With a Substrate Analog Provides Insights Into Substrate Recognition and Raises Questions Regarding Which Metal Cofactors Are Bound in the Enzyme Active Site. Eric Montemayor, Jonathan Schuermann, Alexander Taylor, Scott Stevens, John Hart.

**11:30-11:50am** **01.03.7**
Neutron Crystal Structures of Human Carbonic Anhydrase II at Different Ph Reveal Implications for Catalysis. Zoe Fisher, Andrey Kovalevsky, Marat Mustyakimov, John Domsic, Robert McKenna, David Silverman, Paul Langan.

**11:50-12:10pm** **01.03.6**
Molecular Basis of 1,6-Anhydro Bond Cleavage and Phosphoryl Transfer by Pseudomonas Aeruginosa 1,6-Anhydro-N-Acetylmuramic Acid Kinase. John-Paul Bacik, Garrett Whitworth, Keith Stubbs, Anuj Yadav, Dylan Martin, Ben Bailey-Elkin, David Vocadlo, Brian Mark.

## 05.01 Cool Structures

**Chair: Allen Oliver**
**Maurepas**

**09:00-09:15am** **05.01.1**
Solid-State Structure Determination of Water-Soluble Iridium Half-Sandwich Complexes for Catalytic Water Oxidation. Nathan Schley, James Blakemore, Christopher Incarvito, Gary Brudvig, Robert Crabtree.

**9:15-09:30am 05.01.2**
Pulling Out All Stops: Refinement of a Tricky Crystal Structure. Peter Mueller.

**09:30-09:45am 05.01.3**
Three Strikes and You're Out? Patrick Carroll.

**09:45-10:00am 05.01.4**
Single Crystal Diffraction and Inelastic Neutron Scattering Studies of Ruthenium-Dihydrogen Complexes. Alberto Albinati, Silvia Rizzato, Peter Georgiev, Sax Mason, Jacques Ollivier.

**10:00-10:30am** Coffee break

**10:30-10:45am 05.01.5**
B-Iodinated O-Carboranes: C-H---I Hydrogen Bonding, Absolute Structure Determination and Merohedral Twinning in Space Group P41. Yulia Sevryugina, Alexander V. Safronov, M. Frederick Hawthorne, Charles F. Campana.

**10:45-11:00am 05.01.6**
Three Polymorphs Or How to Grow Crystals From a Melt. Ilia Guzei, Erica Gunn, Lara Spencer, Jennifer Schomaker, Jared Rigoli.

**11:00-11:15am 05.01.7**
Broad Neutralization of Influenza Virus and Implications for a Universal Flu Vaccine . Ian Wilson, Damian Ekiert, Gira Bhabha, Cyrille Dreyful.

**11:15-11:30am 05.01.8**
Structure and Disorder in K4V(NCS)6 'x(OCMe2). Saul Lapidus, Kevin H. Stone, Endrit Shurdha, Joel S. Miller, Peter W. Stephens.

**11:30-11:45am 05.01.9**
Direct Detection of Hydrogen Atoms and Visualization of Hydrogen Bonds in Enzymes. Andrey Kovalevsky, Leif Hanson, Zoe Fisher, Marat Mustyakimov, Sax Mason, Trevor Forsyth, David Keen, Paul Langan.

**11:45-12:00pm 05.01.10**
Ordered Surface Waters Bind Antifreeze Proteins to Ice. Peter L. Davies, Robert L. Campbell, Christopher P. Garnham.

## 07.01 Fast Science

Chair: Tim Graber & Marco Cammarata
D2-D3

**09:00-09:30am 07.01.1**
Picosecond Pump-Probe X-Ray Liquidography (Solution Scattering) to Probe Solution-Phase Structural Dynamics. Hyotcherl Ihee.

**09:30-10:00am 07.01.2**
Time Resolved Crystallographic Analysis of Cooperative Ligand Binding and Ligand Migration in a Dimeric Hemoglobin. William Royer, James Knapp, Zhong Ren, Vukica Srajer.

**10:00-10:30am** Coffee Break

**10:30-11:00am 07.01.3**
Visualizing Sub-Nanosecond Structural Dynamics With Time-Resolved Diffraction and XAFS at the Photon Factory Advanced Ring. Shin-ichi Adachi.

**11:00-11:30am 07.01.4**
Five Dimensional Crystallography. Marius Schmidt, Shailesh Triphathi, Namrta Purwar, Vukica Srajer, Robert Henning, Tim Graber.

**11:30-12:00pm 07.01.5**
First Hard X-Ray Beamline at FEL Sources, Performances and First Experiments in XPP (LCLS/SLAC). Marco Cammarata, David Fritz.

## 08.08 The Devil is in the Details: Local Structure and Diffuse Scattering

Chair: Karena Chapman
D1

**09:05-09:30am 08.08.1**
*In situ* X-Ray Diffraction Studies of Medical Gases Adsorbed in Metal-Organic Frameworks. Phoebe Allan, Karena Chapman, Peter Chupas, Catherine Renouf, Simon Teat, Bo Xiao, Russell Morris.

**09:30-09:45am 08.08.2**
Unusual Effect of Pressure on the Coefficient

of Thermal Expansion for Tao2F: a Zero Expansion Material? Benjamin Greve, Mehmet Centikol, Angus Wilkinson.

**09:45-10:00am** **08.08.3**
Multi-Step Growth of Silver Nanoparticles on a Porous Zeolite. Haiyan Zhao, Karena Chapman, Tina Nenoff, Peter Chupas.

**10:00-10:30am** Coffee Break

**10:30-10:55am** **08.08.4**
Incipient Ferroelectricity in Thermoelectric Lead Telluride. Emil Bozin, Christos Malliakas, Petros Souvatzis, Thomas Proffen, Nicola Spaldin, Mercouri Kanatzidis, Simon Billinge.

**10:55-11:10am** **08.08.5**
*In situ* Pair Distribution Function (PDF) and X-Ray Diffraction (XRD) Studies of Conversion Reactions With Lithium in Bismuth Oxyfluorides. Olaf Borkiewicz, Olaf Borkiewicz, Karena Chapman, Lin-Shu Du, Andrew Gmitter, Glen Amatucci, Clare Grey, Peter Chupas.

**11:10-11:35am** **08.08.6**
3D-PDF Analysis of Single Crystal Diffuse Scattering. Thomas Weber.

**11:35-11:50am** **08.08.7**
Towards the Development of a General Protocol for Modeling Diffuse Scattering of Disordered Materials: Quantitative Structure Analysis of the Disordered Up-Conversion Host Compound Nalaf4. Tara Michels-Clark, Michal Chodkiewicz, Christina Hoffmann, Jorg Hauser, Anthony Linden, Vikie Lynch, Thomas Weber, Hans-Beat Borgi.

**11:50-12:00pm** **08.08.8**
Precipitation and Growth of Nanostructured LaF3 in Glass Ceramics: Multiple Length-Scale Materials. Katharine Page.

## 07.02 Maximizing the Scientific Results of Your Synchrotron Visit

Chair: Stephan Ginell
Maurepas

**01:30-02:00pm** **07.02.2**
The New SSRL BL12-2 Micro-Focus Facility. Aina Cohen, Graeme Card, Pete Dunten, Thomas Eriksson, Ana Gonzalez, Dan Harrington, Irimpan Mathews, Scott McPhillips, Jinhu Song, Michael Soltis.

**02:00-02:30pm** **07.02.3**
Better Data With PILATUS and MYTHEN Detectors. Clemens Schulze-Briese.

**02:30-03:00pm** **07.02.4**
Vector Scanned Microcystallographic Data Collection Techniques. Malcolm Capel, Frank Murphy.

**03:00-03:30pm** Coffee Break

**03:30-04:00pm** **07.02.5**
Isomorphous Replacement From Selenomethionine-Containing Proteins Using UV-Induced Radiation Damage. Daniele de Sanctis, Santosh Panjikar, Paul Tucker.

**04:00-04:30pm** **07.02.6**
Beyond Pushing Buttons: Strategy for Synchrotron High Resolution Data Collection at Room Temperature. Andre Mitschler, Alberto Podjarny, Christophe Mueller-Dickmann, Alexandre Popov.

**04:30-05:00pm** **07.02.7**
Evolving Crystallographic Tools and Techniques at GM/CA Cat That Target Challenging Samples. Craig Ogata, Ruslan Sanishvili, Mark Hilgart, Sergey Stepanov, Michael Becker, Venugopalan Nagarajan, Shenglan Xu, Oleg Makarov, Janet Smith, Robert Fischetti, Sudhir Pothiineni, Derek Yoder, Stephen Corcoran.

## 08.09 Structural Enzymology III - Biology

Chair: Michael Murphy
D2-D3

**01:30-02:05pm** **08.09.1**
Alleviating Anticancer Drug Toxicity by Inhibiting a Bacterial Enzyme. Matthew Redinbo, Bret Wallace.

**02:05-02:40pm** **08.09.2**
Resisting Antibiotic Resistance: Structural Studies of Antibiotic Resistance Enzymes. Albert Berghuis, Desiree Fong, Magdalena Korczynska, Oliver Baettig.

**02:40-03:00pm** **08.09.3**
A Structural Model for Binding of the Serine-Rich Repeat Adhesin GspB to Host Carbohydrate Receptors. Tasia Pyburn, Barbara Bensing, Yan Xiong, Bruce Melancon, Thomas Tomasiak, Victoria Yankovskaya, Gary Cecchini, Gary Sulikowski, Paul Sullam, Tina Iverson, Nicholas Ward, Kevin Oliver.

**03:00-03:30pm** Coffee Break

**03:30-04:05pm** **08.09.4**
A Structural Paradigm for Host Cell Invasion by Apicomplexan Parasites. Martin Boulanger, Michelle Tonkin, Magali Roques, Maryse Lebrun.

**04:05-04:30pm** **08.09.5**
Structural Insights Into Iron Pirating by *Pathogenic neisseria*. Nicholas Noinaj.

**04:30-04:55pm** **08.09.6**
The Structure and Mechanism of Conjugative Plasmid pCU1 Relaxase. Rebekah Nash, Franklin Niblock, Matthew Redinbo.

## 08.10 Educational Inspiration: Crystallographic Teaching Techniques

Chair: Amy Sarjeant
Borgne

**01:25-01:50pm** **08.10.1**
What's All This MoOing About? David Watkin.

**01:50-02:15pm** **08.10.2**
Visualizing Symmetry and Chemical Structure in the Undergraduate Curriculum. Dean Johnston.

**02:15-02:35pm** **08.10.3**
You Can Put It on Your Resume! Publishing Crystal Structures in Collaboration With Undergraduates. Joseph Tanski.

**02:35-03:00pm** **08.10.4**
Teaching Crystallography at MIT. Peter Mueller.

**03:00-03:30pm** Coffee Break

**03:30-03:55pm** **08.10.5**
Teaching and Learning Macromolecular Crystallography: Tools, Tips and Experiences Acquired Over 25+ Years. William Furey.

**03:55-04:20pm** **08.10.6**
Crystal Cookery - Using High-Throughput Technologies and the Grocery Store as a Teaching Tool. Edward Snell, Joseph R. Luft, Jennifer R. Wolfley, M. Elizabeth Snell, Stephen A. Potter.

**04:20-04:45pm** **08.10.7**
Crystallography Experiments for an Undergraduate Laboratory. Nigam Rath, Christopher Spilling, Stephen Holmes.

**04:45-05:05pm** **08.10.8**
Making Movies of Solid-State Transformations: Professor Inspires Students and Students Inspire Professor. Bruce Foxman, Aaron R. Gell, Shai R. Posner.

# TUESDAY, MAY 31

## 08.11 Diffraction Studies of Industrial Materials

**Chairs: Yan Gao & Bryan Chakoumakis**
**D1**

**01:30-02:00pm** **08.11.1**
Addressing Industrial Challenges With High-Energy X-Rays. Jonathan Almer.

**02:00-02:15pm** **08.11.2**
Real Time High Energy X-Ray Diffraction Studies of Oil Well Cement Hydration Under Down Hole Conditions. Angus Wilkinson, Angus Wilkinson, Andrew Jupe, Gary Funkhouser.

**02:15-02:45pm** **08.11.3**
Strain- and Phase-Mapping With High-Energy Synchrotron X-Rays at the X17B1 Beamline of the National Synchrotron Light Source. Zhong Zhong, Y. Gao, J. Rijssenbeek, G. Zappi, J. Skaritka, K. Akdogan, M. Croft, A. Ignatov, T. Tsakalakos.

**02:45-03:00pm** **08.11.4**
Crystal Structure of Monoclinic Sr24 Ca06 Al2 O6. James Kaduk, Winnie Wong-Ng, Joseph Golab.

**03:00-03:30pm** Coffee Break

**03:30-04:00pm** **08.11.5**
Microelectronics Materials and Synchrotron X-Rays: Metal Silicide Research by IBM at the NSLS. Jean Jordan-Sweet, Christian Lavoie.

**04:00-04:15pm** **08.11.6**
Analysis of the Microstructure of Severely Deformed Ti by X-Ray Diffraction and Ebsd. Natalia De Vincentis, Anibal Mendes Filho, Maurizio Ferrante, Martina Avalos, Raul Bolmaro.

**04:15-04:45pm** **08.11.7**
Providing Solutions for Industry - the Vulcan Diffractometer at the SNS. Xun-Li Wang, Ke An, Alexandru D. Stoica, Harley D. Skorpenske, Dong Ma, Ling Yang, Xun-Li Wang.

*EVENING SESSIONS*

## 6.02 Would You Publish This?

Chair: Carla Slebodnick
Borgne 07:00pm
*sponsored, in part, by Agilent Technologies, Crystallographic Resources, Inc., and Ellen Mathena*

**06.02.2**
Tethered Bis-Phenanthroline Copper Complexes: Dimers, Trimers, Polymers. Allen Oliver, Luis Lemus, Graham Lappin.

**06.02.3**
A Nasty Chain of Events. Amy Sarjeant, Charlotte Stern, Zhixue Zhu, J. Fraser Stoddart.

**06.02.4**
Crystal Structure of a Dimerized Pyridal Polyazine Complex With Photochemical Properties. Muhammed Yousufuddin, Joseph Aslan, Frederick MacDonnell.

**06.02.5**
What If We Cannot Balance the Charges? Khalil A. Abboud, Tu Nguyen, Constantinos Efthymiou, George Christou.

**06.02.6**
My Bionic Crystal Structure: How I Put a Buckyball in a Buckybowl (With a Lot of Help!). Louise N. Dawe, Jason I. Mercer, Huu-Ahn Tran, Tayel AlHujran, Edward A. Jackson, Lawrence T. Scott, Paris E. Georghiou.

**06.02.7**
A Case of a Poorly Diffracting Crystal. Larry Falvello.

## Panel Discussion: Industrial Access to National User Facilities

Chair: Jim Kaduk
D1 07:30pm

Dean Myles (SNS/ORNL)
Dennis Mills (APS/ANL)
Jun Wang (NSLS/BNL)
Michel Fodje (CLS)

| | | |
|---|---|---|
| Registration Desk | 07:30am | Napolean Foyer |
| Speaker Ready Room | 07:30am | Oakley, 4th floor |
| Council Meeting Room | 07:30am | Nottoway, 4th floor |
| Industrial SIG Meeting | 12:00pm | D2-D3 |
| Neutron/Materials/Powder Joint SIG Meeting | 12:00pm | D1 |
| Small Angle Scatteirng SIG Meeting | 12:00pm | Maurepas |
| **Annual Award Banquet** (ticket required) | | |
| Cash Bar 06:30-07:30pm Dinner | 07:30-10:30pm | Armstrong Ballroom, 8th floor |

## SP.04 Fankuchen Award

**Award presentation to David Watkin by President Thomas Koetzle .**
**D2-D3**

**08:00-08:50am** **SP.04.1**
Crystallography - Is the Gold Standard Getting Tarnished? David Watkin.

## 01.04 Membrane Protein Crystallization

Chair: Michael Wiener
Borgne

**09:00-09:30am** **01.04.1**
High Throughput Production of Membrane Proteins for Crystallography. NYCOMPS, Brian Kloss, Renato Bruni, Marco Punta, Burkhard Rost, Arianne Morrison, Filippo Mancia, Larry Shapiro, Wayne Hendrickson.

**09:30am-10:00am** **01.04.2**
Membrane Protein Pre-Crystallization Screening. Michael Wiener, James Vergis, Michael Purdy, Rachel Reuther.

**10:00-10:30am** Coffee break

**10:30-10:45am** **01.04.3**
Expanding Crystallization Optimization Capacity Using Alchemist-tm DT. Jian Xu, Matthew Lundy, Michael Willis.

**10:45-11:00am** **01.04.4**
A Fast and Fully Automated Solution for Lipidic Cubic Phase (LCP) Screening Using Mosquito LCP. Joby Jenkins, Patricia Edwards, Rob Lewis, Joanne Franklin.

**11:00-11:30am** **01.04.5**
Structure-Function Studies of Family B GPcrs and Their Signaling Complexes. Hilary Stevenson, Qiangmin Zhang, Flippo Pullara, Guillermo Calero.

**11:30-12:00pm** **01.04.6**
Current Progress on Membrane Protein Femtosecond Nanocrystallography. Mark Hunter, John Spence, Henry Chapman, Rick Kirian, Tom White, Uwe Weierstall, Anton Barty, Dan DePonte, R. Bruce Doak, Petra Fromme.

## 04.03 Information in SAXS/WAXS Data

Chair: Hiro Tsuruta & Lee Makowski
Maurepas

**09:00-09:30am** **04.03.1**
Structural Determinants of Multidomain Complexes: Integrating SAXS and Biophysical Computations. Sichun Yang.

**09:30-10:00am** **04.03.2**
Robust, High-Throughput Solution Structural Analyses by Small Angle X-Ray Scattering (SAXS). Michal Hammel.

**10:00-10:30am** Coffee Break

**10:30-11:00am** **04.03.3**
Picosecond Time-Resolved SAXS/WAXS Studies of Proteins: Probing Structural Dynamics in Real Time. Philip Anfinrud, Friedrich Schotte, Hyun Sun Cho, Naranbaatar Dashdorj, William Royer, Henning Robert, Graber Timothy.

**11:00-11:30am** **04.03.4**
Snapshot SAXS for *ab initio* Imaging From Spatial Correlations. Richard Kirian, Kevin Schmidt, Dilano Saldin, John Spence.

**11:30-12:00pm 04.03.5**
DNA Conformations in Mismatch Repair Seen in Solution by X-Ray Scattering From Gold Nanocrystals. Greg Hura, Shelley Claridge, Marc Mendillo, Christopher Putnam, Richard Kolodner, A. Paul Alivisatos, John Tainer.

## 05.02 Modern Aspects of Crystal Engineering I

Chair: Travis Holman
D2-D3

**09:00-09:30am 05.02.1**
*Ab initio* Crystal Structure Prediction: Developments for Flexible Molecules and Applications to Porous Materials. Graeme Day.

**09:30-10:00am 05.02.2**
Utilizing Self-Assembling Macrocycles to Generate Functional Porous Crystals. Linda Shimizu, Sandipan Dawn, Mahender Dewal, Kinkini Roy, Yuewen Xu, Jun Yang.

**10:00-10:30am** Coffee Break

**10:30-11:00am 05.02.3**
Towards An Understanding of Molecular Crystals: Challenges, Strategies and Solutions. Kenneth D.M. Harris.

**11:00-11:20am 05.02.4**
Sulfonamidecinnamic Acids: Merging Supramolecular Asymmetry and Programmed Crystal Reactivity. Kraig Wheeler.

**11:20-11:35am 05.02.5**
Supramolecular Catalysis in the Organic Solid State. Jelena Stojakovic, Anatoliy Sokolov, Dejan-Kresimir Buçar, Jonas Baltrusaitis, Sean Gu, Leonard MacGillivray.

**11:35-11:50am 05.02.6**
Guest-Free Cavitands: Low Packing Fraction Materials. Christopher Kane, K. Travis Holman.

**11:50-12:00pm 05.02.7**
Polymorphism of the Secondary Explosive RDX Revisited. Ilana Goldberg, Jennifer Swift.

**12:00-01:30pm** Lunch break

**01:30-02:00pm 05.02.8**
Co2 Capture in Amine Modified Metal Organic Frameworks. George Shimizu, Ramanathan Vaidhyanathan, Simon Iremonger, Isaac Martens.

**02:00-02:30pm 05.02.9**
Pore Expansion and Contraction of Metal-Organic Frameworks Upon Adsorption. Praveen Kumar Thallapally, Benard McGrail.

**02:30-03:00pm 05.02.10**
Engineering Crystals for Energy and Environmental Applications. Radu Custelcean.

**03:00-03:30pm** Coffee Break

**03:30-03:45pm 05.02.12**
A Series of Uranyl-4,4'-Biphenyldicarboxylates: Synthesis, Structure and Fluorescent Properties. Paula Cantos, Christopher Cahill.

**03:45-04:00pm 05.02.13**
Sonochemical Preparation of Pharmaceutical Nano-Cocrystals. John R.G. Sander, Dejan-Kresimir Buçar, Rodger F. Henry, Geoff G. Z. Zhang, Leonard R. MacGillivray.

**04:00-04:30pm 05.02.14**
Thermodynamic of Co-Crystal Formation and An Efficient Screening Method Based on Solution-Mediated Phase Transformation (SMPT). Geoff G.Z. Zhang.

**04:30-04:50pm 05.02.15**
Crystal Engineering of Quaternary Ammonium Salts of a Morphinan Opoid Modulator: Impact of Hydration Behavior on Form Selection. Mark Oliveira, Magali Hickey, Mark Tawa, Julius Remenar, Carlos Sanrame, Cherie Guo, Kenneth Hardcastle, Bruce Foxman, Orn Almarsson.

**04:50-05:10pm 05.02.16**
The Fascinating World of Tautomers and Their Crystal Structures. AuroraJ. Cruz-Cabeza, Colin R. Groom.

## 08.13 Evolution of Powder Diffraction Software: In Honor of Lachlan Cranswick

Chair: Peter Stephens
D1

**09:10-09:35am** **08.13.1**
CMPR, EXPGUI and Lachlan. Brian Toby.

**09:40-10:00am** **08.13.2**
Visualization of Diffraction Volumes of Polycrystalline Materials Using Max3D. Jim Britten, Weiguang Guan, Victoria Jarvis.

**10:00-10:30am** Coffee Break

**10:30-10:50am** **08.13.3**
SRREAL - An Open-Source Toolbox for Real-Space Structure Analysis. Pavol Juhas, Christopher Farrow, Simon Billinge.

**10:55-11:15am** **08.13.4**
Method Development and Applications of Structure Envelope Generation for Structure Solution of MOF Materials. Andrey A. Yakovenko, Joseph H. Reibenspies, Nattamai Bhuvanesh, Hong-Cai Zhou.

**11:20-11:40am** **08.13.5**
The Impact of the Fundamental Parameters Approach on NIST Powder Diffraction SRMS. Jim Cline, Katherine Mullen, David Black, Donald Windover, Albert Henins.

**11:45-12:05pm** **08.13.6**
Software Enabling Science: Nanostructure From Diffraction. Simon Billinge.

## 03.01 Challenges and Opportunities in Structure Based Drug Discovery

Chair: Nickolay Chirgadze
Maurepas

**01:30-02:00pm** **03.01.1**
Diversity Assessment and Design of Efficient Fragment Libraries Using the PDB and Enumeration of Protein Binding Motifs. John Badger.

**02:00-02:30pm** **03.01.2**
Discovery of Novel Fragment Inhibitors of Acetyl Coa Carboxyltransferase. Felix Vajdos, Marie Anderson, Kris Borzilleri, Venkataraman Thanabal.

**02:30-03:00pm** **03.01.3**
Managing 2D and 3D Ligand Fragments From Disparate Large Resources for Structure Based Drug Discovery. Talapady Bhat.

**03:00-03:30pm** Coffee Break

**03:30-04:00pm** **03.01.4**
Structures of Human Hepatitis C Virus Ns5B Polymerase With Inhibitors Bound to the P495 and Primer Grip Sites Reveal Enzyme Flexibility. Steven Sheriff, Changhong Wan, Kevin Kish, Daniel Camac, Chong-Hwan Chang, Brett Beno, Xiaofan Zheng, Robert Gentles, Min Ding, Louis Chupak, Paul Morin, Mark Witmer, Thomas Hudyma, Feng He, Michael Poss, John Kadow, Karen Rigat, Ying-Kai Wang, Robert Fridell, Julie Lemm, Dike Qiu, Mengping Liu, Stacey Voss, Lenore Pelosi, Susan Roberts, Min Gao, Jay Knipe.

**04:00-04:30pm** **03.01.5**
A Novel Strategy for Studying the X-Ray Crystal Structures of Nucleic Acid-Small Molecule Complexes. Jia Sheng, Jozef Salon, Julianne Caton-Williams, Abdalla Hassan, Wen Zhang, Jianhua Gan, Lina Lin, Huiyan Sun, Zhen Huang.

**04:30-05:00pm** **03.01.7**
Small Molecules in Protein Structures. David Cooper, Maksymilian Chruszcz, Marcin Cymborowski, Przemek Porebski, Igor Shumilin, Heping Zheng, Wladek Minor.

## 08.12 Macromolecular Assemblies

Chair: Chris Hill
Borgne
*sponsored, in part, by Area Detector Systems and Rigaku*

**01:30-02:06pm** **08.12.1**
Structural Basis for Nucleosome Recognition by the RCC1 Chromatin Factor. Song Tan, Ravindra Makde, Joseph England, Jiehuan Huang, Hemant Yennawar.

**02:06-02:24pm** **08.12.2**
Structure of Hibiscus Latent Singapore Virus by Fiber Diffraction: a Non-Conserved His122 Contributes to Coat Protein Stability. Kunchithapadam Swaminathan, Sunil Kumar Tewary, Toshiro Oda, Amy Kendall, Wen Bian, Gerald Stubbs, Sek-Man Wong.

**02:24-02:42pm** **08.12.3**
Structural Insights Into Holoenzyme Assemblies and Substrate Preferences of Biotin-Dependent Carboxylases. Christine Huang, Liang Tong.

**02:42-03:00pm** **08.12.4**
Structural Basis for Cooperative Recognition of RNA by NUSB and NUSE During Transcription Antitermination. Jason R. Stagno, Amanda S. Altieri, Mikhail Bubunenko, Sergey G. Tarasov, Jess Li, Donald L. Court, R. Andrew Byrd, Xinhua Ji.

**03:00-03:30pm** Coffee Break

**03:30-04:06pm** **08.12.5**
Structure of the HIV Capsid. Owen Pornillos, Barbie Ganser-Pornillos, Mark Yeager.

**04:06-04:24pm** **08.12.6**
The Crystal Structure of a Novel Scaffolding Unit of the Nuclear Pore Complex: a Low-Resolution Odyssey. Silvija Bilokapic, Kanagalaghatta Rajashankar, Thomas Schwartz.

**04:24-05:00pm** **08.12.7**
Dynamic Structural Mechanisms Underlying Ubiquitin-Like Protein Conjugation. Brenda Schulman.

## 08.14 Diffraction Studies of Magnetic Materials

Chair: Clarina De La Cruz
D1

**01:30-01:55pm** **08.14.1**
Magnetic and Structural Properties of Iron-Based Superconductors. Jeffrey Lynn.

**01:55-02:20pm** **08.14.2**
Superconductivity in Iron Chalcogenides. Mark Green.

**02:20-02:35pm** **08.14.3**
Small Angle Neutron Scattering Studies of Kfe2As2. Lisa DeBeer-Schmitt, Hazuki Kawano-Furukawa, Alistair Cameron, Richard Heslop, Jon White, Charlotte Bowell, Ken Littrell, Jorge Gavilan, E. M . Forgan.

**02:35-03:00pm** **08.14.4**
On the Superspace Symmetry of Incommensurate Magnetic Structures and its Applications. Manuel Perez-Mato, Jose Luis Ribeiro, Vaclav Petricek, Mois Aroyo.

**03:00-03:30pm** Coffee Break

**03:30-03:55pm** **08.14.5**
Geometrically Frustrated Magnetism - a New Route to Room Temperature Spintronics. Andrew Wills, Laura Fenner.

**03:55-04:20pm** **08.14.6**
Twist the Magnetism in the Multiferroic Mn1-xmMexWO4 (Me: Fe, Zn, Co). Feng Ye, Songxue Chi, Huibo Cao, Jaime Fernandez-Baca, Y.-Q. Wang, Bernd Lorenz, C.W. Chu.

**04:20-04:35pm** **08.14.7**
Phase Separation and Phase Transitions in Multiferroic K3Fe5F15. Sandra Reisinger, Philip Lightfoot, Marc Leblanc, Anne-Marie Mercier.

**04:35-05:00pm** **08.14.8**
Coupling of Magnetic and Ferroelectric Hysteresis by a Multi-Component Magnetic Structure in Mn2Geo4. Jonathan White, T. Honda, T. Kimura, Ch. Niedermayer, O. Zaharko, A. Poole, B. Roessli, V. Yu. Pomjakushin, M. Kenzelmann.

**05:00-05:15pm** **08.14.9**
Elastic Neutron Scattering Study of Single Crystal BaMnO3 and its Doped Compounds. Songxue Chi, Feng Ye, Huibo Cao, Jaime Fernandez-Baca, Gang Cao.

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|---|---|---|
| Registration Desk | 07:30am | Napolean Foyer |
| Speaker Ready Room | 07:30am | Oakley, 4th floor |
| Council Meeting Room | 07:30am | Nottoway, 4th floor |

## SP.05 Plenary Lecture:
**Ned Seeman, New York University**
**D2-D3**

**08:00-08:50am** **SP.05.1**
DNA: Not Merely the Secret of Life. Ned Seeman.

## 08.15 Data Processing with the Pros
Ed Collins & Andy Torelli
Borgne
*sponsored, in part, by DECTRIS, Ltd., Rayonix and Rigaku*

**09:00-09:30am** **08.15.1**
Data Processing With XDS. Kay Diederichs.

**09:30-10:00am** **08.15.2**
Mosflm & iMosflm. Harry Powell, Andrew Leslie.

**10:00-10:30am** Coffee Break

**10:30-11:00am** **08.15.3**
Professional Results From Diffraction Images With D*Trek. James Pflugrath.

**11:00-11:30am** **08.15.4**
Tools for Working With Problematic Protein Crystals in the Proteum Software Suite. Matthew Benning.

**11:30-12:00pm** **08.15.5**
Processing "Difficult" Data With Hkl-2000/Hkl-3000. Wladek Minor, Marcin Cymborowski, Zbyszek Otwinowski, Maksymilian Chruszcz, Dominika Borek.

## 08.16 Earth Materials
Chairs: John Parise & Ian Swainson
D1

**09:00-09:20am** **08.16.1**
Sulfate Minerals in Extreme Environments: From Toxic Mine Waste to the Salars of the High Andes to the Surface of Mars. Ron Peterson.

**09:20-09:40am** **08.16.2**
High Pressure Transformations in Clathrate Materials. Chris Tulk, Dennis Klug, Antonio Moreira dos Santos, Jorg Neuefeind, Veijo Honkimaki, Jamie Molaison, Neelam Pradhan.

**09:40-10:00am** **08.16.3**
New Insights Into the Structure of Amorphous Calcium Carbonate From Neutron and X-Ray Scattering Investigations. Alejandro Fernandez-Martinez, Yandi Hu, Young-Shin Jun, Glenn Waychunas.

**10:00-10:30am** Coffee Break

**10:30-10:45am** **08.16.4**
Mendeleevite-(Ce), a New Mineral and a Potential New Microporous Material. Elena Sokolova, Frank Hawthorne, Leonid Pautov, Atali Agakhanov, Vladimir Karpenko.

**10:45-11:00am** **08.16.5**
Short-Range Constraints on Chemical and Structural Variations in Bavenite. Frank Hawthorne, Aaron Lussier.

**11:00-11:15am** **08.16.6**
Braitschite: a Crystallographic Challenge and a Structure to Show for It. Clare Rowland, Christopher Cahill, Jeffrey Post.

**11:15-11:30am** **08.16.10**
*In-situ* Study of Kerogen Release and Metamorphism in Oil Shale by SANS. Kenneth

Littrell, Gernot Rother, David Cole, Larry Anovitz, Lisa DeBeer--Shmitt.

**11:30-11:45am 08.16.11**
X-Ray Analysis of Ferrous and Manganese-Ferrous Ores From Lakes and Marshes of Vologda Region. Nikolay Fedorchuk, Anton Chuev, Anatoly Pichurin.

**11:45-12:00pm 08.16.12**
Hydrated Sodium-Magnesium Sulfate Minerals Associated With Inland Saline Systems. Evelyne Leduc, R.C. Peterson.

## 08.17 Combined Techniques for Determining the Structure of Complexes and RNAs in Solution

Chairs: Yun-Xing Wang & John Tainer Maurepas

**09:00-09:25am 08.17.1**
Accurate Conformations, Assemblies and Structures of Macromolecules in Solution by X-Ray Scattering (SAXS) Combined With Crystallography. John Tainer, Robert Rambo, Greg Hura, Michal Hammel.

**09:30-09:55am 08.17.2**
Solution Structure of the 128 kDa Enzyme I Dimer from *Escherichia coli* and its 146 kDa Complex With HPr Using Residual Dipolar Couplings and Small and Wide Angle X-Ray Scattering. Marius Clore, Yuki Takayama, Alexander Grishaev, Jeong-Yong Suh, Charles Schwieters.

**10:00-10:25am 08.17.3**
Combined Use of SAXS and NMR for Structural Determination of Large RNAs and RNA Complexes in Solution. Xiaobing Zuo, Jinbu Wang, Ping Yu, Yun-Xing Wang.

**10:30-10:55am 08.17.4**
Solution X-ray Scattering Data in Structure Determination: Application to Macromolecular Assemblies. Alexander Grishaev, Charles Schwieters, Marius Clore, Ad Bax.

**11:05-11:20am 08.17.5**
Quantitative Assessments of Flexibility and Validation of Biopolymer Models Using the Porod-Debye Law. Robert Rambo, John Tainer.

**11:25-11:40am 08.17.6**
Integrative Structure Determination of the Components of the Nuclear Pore Complex by X-ray Crystallography, Small Angle X-Ray Scattering, Electron Microscopy, and Comparative Modeling. Seung Joong Kim, Parthasarathy Sampathkumar, Javier Fernandez-Martinez, Jeremy Phillips, Dina Schneidman, Tsutomu Matsui, Hiro Tsuruta, Michael Sauder, Michael Rout, Andrej Sali.

**11:45-12:00pm 08.17.7**
Time-Resolved SAXS Studies Revealed Crucial Roles of Autoproteolysis in a T=4 Virus Maturation. Tsutomu Matsui, John Johnson, Hiro Tsuruta.

**12:05-12:20pm 08.17.8**
Elucidating the Substrate Interaction Mechanism of the Hsp90 Molecular Chaperone. Timothy Street, Laura Lavery, David Agard.

## 08.18 Small Molecule Molecular Machines

Chair: Christopher Incarvito
D2-D3
*sponsored, in part, by Yale University*

**09:00-09:30am 08.18.1**
Mechanical Properties in Supramolecular Assemblies. Jeremiah Gassensmith.

**09:30-10:00am 08.18.2**
Ultra-Fast Rotors for Molecular Machines and Functional Materials Via Halogen Bonding: Crystals of 1,4-Bis(Iodoethynyl)Bicyclo[222] Octane With Distinct Gigahertz Rotation at Two Sites. Cortnie Vogelsberg, Cyprien Lemouchi, Leokadiya Zorina, Sergey Simonov, Patrick Batail, Stuart Brown, Miguel Garcia-Garibay.

**10:00-10:30am** Coffee Break

**10:30-11:00am** **08.18.3**
Towards a Hydrogen Bond Molecular Switch. Carla Daly, Anita R. Maguire, Simon E. Lawrence.

**11:00-11:30am** **08.18.4**
Recent Advances in the Design and Characterization of Amphidynamic Crystals and Molecular Machines. Miguel Garcia-Garibay.

**11:30-12:00pm** **08.18.5**
Copper-Complexed Rotaxane Struts in a Metal-Organic Framework. Gokhan Barin, Ali Coskun, Mohamed Hmadeh, Omar Yaghi, Fraser Stoddart.

## 02.02 General Interest-II

Chair: Allen Oliver
D1

**01:30-01:45pm** **02.02.1**
Applications of Two-Dimensional X-Ray Diffraction on Single-Crystal CCD Instruments. Charles Campana, Baoping Bob He, Brian Jones, Holger Cordes.

**01:45-02:00pm** **02.02.2**
High-Brilliant X-Ray Sources for Chemical and Biological Crystallography in the Home Lab: An Update. Juergen Graf, Carsten Michaelsen, Matthew Benning.

**02:00-02:15pm** **02.02.3**
The WWPDB X-Ray Validation Task Force, Low-Resolution Model Accuracy, and Visualizing Clusters of Local Error. Bradley Hintze, Christopher Williams, Jane Richardson, David Richardson.

**02:15-02:30pm** **02.02.4**
Data Quality in Area Detector Diffraction Experiments. Mathias Meyer.

**02:30-02:45pm** **02.02.5**
Better Instrument Design for Better Data. Michael Ruf, Gary Bryant, Joerg Kaercher, Detlef Bahr, Christoph Ollinger, Brian Michell.

**02:45-03:30pm** Coffee break

**03:30-03:50pm** **02.02.6**
Ribosomal Protein S19, a Rosetta Stone of Speciation. William Duax, Robert Huether, David Dziak.

**03:50-04:20pm** **02.02.7**
Nucleation and Crystallization Kinetics in Powders Probed by Second Order Nonlinear Optical Imaging of Chiral Crystals (SONICC). Garth Simpson.

**04:20-04:30pm** **02.02.8**
Acoustic Liquid Handling Applied to Protein Crystallography--Miniaturizing, Formulating, Transferring, Seeding, Monitoring, & LCP Formation. Joe Olechno, Sammy Datwani, Brent Eaton, Rich Ellson.

**04:30-04:50pm** **02.02.9**
Random Microseeding: a Theoretical and Practical Exploration of the Microseed Matrix Screening (MMS) Method, with New Recommendations for Achieving Crystallization Success. Patrick D. Shaw Stewart, Richard A. Briggs, Stefan A. Kolek, Peter Baldock.

## 08.19 Phasing and Refinement for Dummies: No Book Required

Chairs: Ed Collins & Andy Torelli
Borgne
*sponsored, in part, by Rigaku*

**01:00-02:15pm** **08.19.1**
Automated Processing With Added Value. Clemens Vonrhein, Claus Flensburg, Peter Keller, Wlodek Paciorek, Andrew Sharff, Oliver Smart, Thomas Womack, Gerard Bricogne.

**02:15-03:00pm** **08.19.2**
Picking the Low-Hanging Fruit With SHELXC/D/E. George Sheldrick.

**03:00-03:30pm** Coffee Break

**03:30-04:15pm** **08.19.3**
Macromolecular Refinement Program - REFMAC. Garib Murshudov.

**04:15-05:00pm** **08.19.4**
Crystallographic Structure Solution Using Phenix. Pavel Afonine.

## 08.21 New Bio-Science from Emerging Opportunities and Sources

Chair: Bob Sweet
Maurepas

**01:30-01:53pm** **08.21.1**
Femtosecond Nanocrystallography of Membrane Proteins. Petra Fromme.

**01:53-02:15pm** **08.21.2**
Pushing the Boundaries of Resolution and Accuracy of Macromolecular Structures Using Neutron and X-Ray Diffraction. Julian Chen, Paul Langan, Christina Hoffmann, Stephen Ginell.

**02:15-02:38pm** **08.21.3**
*In situ* Coherent Diffraction Imaging of Cellulose Crystals. Lee Makowski, Jyotsana Lal, Ross Harder, Ian Robinson.

**02:38-03:00pm** **08.21.4**
Neutron Structure of Type-III Antifreeze Protein Leads to a Model of AFP-ICE Interface. Alberto Podjarny, Howard Eduardo, Matthew Blakeley, Michael Haertlein, Isabelle Petit-Haertlein, Andre Mitschler, Stuart Fisher, Alexandra Cousido-Siah, Alexandre Popov, Tania Petrova.

**03:00-03:30pm** Coffee Break

**03:30-03:53pm** **08.21.5**
Combining Joint X-Ray/Neutron Crystallography and Quantum Enzymology (Quene) to Study Enzyme Mechanisms. Andrey Kovalevsky, Matt Challacombe, Nicolas Bock, Zoe Fisher, Marat Mustyakimov, Paul Langan.

**03:53-04:15pm** **08.21.6**
Higher Energy Beamlines, a New Paradigm for Macromolecular Crystallography. Roger Fourme, Eric Girard, Richard Kahn.

**04:15-04:38pm** **08.21.7**
Long-Wavelength Macromolecular Crystallography - Challenges and Opportunities. Armin Wagner.

**04:38-05:00pm** **08.21.8**
Next Generation X-Ray and Neutron Macromolecular Refinement Using a Polarizable Force Field. Timothy Fenn, M.J. Schnieders, M. Mustyakimov, C. Wu, P. Langan, V.S. Pande, A.T. Brunger.

## TR.01/05.01 Transactions continued & More Cool Structures

Morning Chair: Jason Benedict
D2D-3

**01:30-01:50pm** **TR.01/05.01.1**
On the Use of Calculated Adps for Charge-Density Analysis of Normal-Resolution Data. Birger Dittrich.

**01:50-02:10pm** **TR.01/05.01.2**
Thermal Motion in Charge Density Studies Revisited. Alan Pinkerton, Vladimir Zhurov, Elizabeth Zhurova.

**02:10-02:30pm** **TR.01/05.01.3**
Determination of Time-Resolved Structural Changes of Dissolved Molecules With Xfel Radiation. Dilano Saldin, Hin-Cheuck Poon, Marius Schmidt, John Spence.

**02:30-02:45pm** **TR.01/05.01.4**
Thermal and Photocrystallographic Studies on a Nickel-Nitro Complex. Lauren Hatcher, Mark Warren, Paul Raithby.

**02:45-03:00pm** **TR.01/05.01.5**
Use of Imagine for Charge Density Studies. Parthapratim Munshi, Flora Meilleur, Tibor Koritsanszky, Robert Blessing, Bryan Chakoumakos, Dean Myles.

**03:00-03:30pm** Coffee break

**Afternoon Chair: Jeanette Karuse**

**03:30-03:45 TR.01/05.01.6**
The Day I Broke SHELX, and Other Synchrotron Anectdotes. Christine Beavers, Spyros Perlepes, Simon Teat, Marilyn Olmstead, Patrick Gamez.

**03:45-04:00pm TR.01/05.01.7**
Allostery in Human UDP-alpha-D-Glucose 6-Dehydrogenase is Mediated by Packing Defects. Zachary Wood, Renuka Kadirvelraj, Stephen Weitzel, Nicholas Sennet, Samuel Polizzi.

**04:00-04:15pm TR.01/05.01.8**
Crystal Structure of New Superconducting Materials MxFe2-x/2Se2: Twinning vs. Disorder. Peter Zavalij, Mark Green.

**04:15-04:30pm TR.01/05.01.9**
Addressing Data Collection and Structure Solution Challenges From Light-Atom Clathrates With Very Large Z'. Jesse Rowsell, Matthias Zeller, Charles Campana.

**04:30-04:45pm TR.01/05.01.10**
Three New Endohedral Fullerenes, Sm2@C88, Sm2@C90, and Sm2@C92. Marilyn Olmstead, Brandon Mercado, Christine Beavers, Alan Balch, Hua Yang, Ziyang Liu.

**04:45-05:00pm TR.01/05.011**
(1,2,3-Trimethylpyridinium) 2Cu5Cl10-Linear Pentacopper(II) Complexes Crosshatched to Form an Egg-Tray Template. Marcus Bond.

## FRIDAY, JUNE 3

### 2012 Boston Meeting Planning Session

**08:30am** **Grand Chenier, 5th floor**

# POSTER PRIZES

**Pauling Poster Prize, Canadian and IUCr Poster Prize**
The Pauling Poster Prize was established by the ACA, and is supported by member contributions, to honor Linus Pauling. Pauling was one of the pioneers in American structural research and was very supportive of the ACA. At each annual meeting, the five best graduate or undergraduate poster presentations receive Pauling awards. Each award consists of $200, a complimentary banquet ticket, and a copy of a Linus Pauling book. An additional Pauling Prize sponsored by the Canadian Division of the ACA and the Canadian National Committee of the IUCr, will be given to the highest ranked graduate or undergraduate poster from a Canadian laboratory. Honorable mention awards for this prize are also made; they consist of a complimentary banquet ticket. IUCr Poster Prize: The IUCr Executive Committee is pleased to continue a series of IUCr awards presented at meetings of the regional affiliates and national crystallographic associations. The award is complimentary online access to all IUCr journals for one year or a complimentary volume of International Tables or other IUCr publication.

**Journal of Chemical Crystallography Prize**
The best student poster presentation in the area of chemical crystallography or small molecule structure determination and analysis is sponsored by Springer's Journal of Chemical Crystallography <www.springer.com> . The winner will receive their personal choice of books from Springer's extensive portfolio of titles.

**RCSB Protein Data Bank Poster Prize**
This prize recognizes a student poster presentation involving macromolecular crystallography. The award will be two educational books that will be mailed to the winner after the meeting. An announcement will appear on the RCSB PDB website and newsletter. For more information, see www.rcsb.org/pdb

**CrystEngComm Poster Prize**
CrystEngComm (published by the Royal Society of Chemistry) is very pleased to sponsor a prize to be awarded to the best student poster presentation in the area of crystal engineering /supramolecular chemistry. The winner will receive an RSC book voucher and an announcement will be posted on the CrystEngComm website (http://www.rsc.org/Publishing/Journals/CE/about.asp) shortly after the conclusion of the ACA meeting.

**Oxford Cryosystems Low Temperature Poster Prize**
This prize is open to all participants and is awarded to the best poster describing work in low temperature crystallography. The winner will receive a cash prize donated by Oxford Cryosystems, Inc.

**American Chemical Society's International Year of Chemistry Poster Prize**
The ACA is happy to announce a special poster prize for 2011- The American Chemical Society's International Year of Chemistry Poster Prize. The award (an IPOD-Nano) is intended to recognize an outstanding poster contribution from a junior scientist (undergrad, grad or post-doc) in the area of Chemical Crystallography, or who has used crystallography to solve a chemical problem. The ACA gratefully acknowledges the American Chemical Society (www.acs.org/international) for this opportunity.

## POSTER HANGING INSTRUCTIONS

Posters beginning with **S** should be assembled before 05:00pm on Sunday and be removed at the conclusion of the poster session at 7:30pm.

Posters beginning with **M** should be assembled before 05:00pm on Monday and be removed at the conclusion of the poster session at 7:30pm.

Posters beginning with **T** should be assembled before 05:00pm on Tuesday and be removed at the conclusion of the poster session at 7:30pm.

**Please be present at your poster from 5:30 - 7:30pm on the day to which you are assigned and remove your poster at the end of the session.**

## Sunday Posters

S01
Growing Lysozyme Crystals for Neutron Diffraction Beamlines. Elena Magay, Yoon Tae-Sung.

S03
X-Ray Structure and Dft Calculations of Methyl 5-Acetyl-2-Hydroxybenzoate. H.C. Devarajegowda, Waleed Fadl Ali Al-eryani, Ravish Sankolli, Suresh Babu Vepuri, M. Vinduvahini, H.K. Arunkashi.

S04
Crystal Structure of N-(4-Heptylphenyl) Acetamide. M VINDUVAHINI, H.C. Devarajegowda, Fadl Ali Al-eryani Waleed, H.T. Srinivasa.

S05
Synthesis and Crystal Structure of the Double Perovskites Alabsbo6, With a = Ba2+ and Pb2+ and B = Mn2+, Co2+, Ni2+, Cu2+ and Zn2+. Diego Franco, Cecilia Blanco, Raul Carbonio.

S06
The Role of Ing4 and Ing5 Tumor Suppressors in Chromatin Remodeling and Disease. Karen Glass, Nehme Saksouk, Pedro Pena, Kyle Johnson, Tiffany Hung, Xiang-Jiao Yang, Jacques Cote, Or Gozani, Tatiana Kutateladze.

S08
Angular Tetrachloro[6]Phenylene: a Step Toward Circular Phenylenes. Alexandr Fonari, Tatiana Timofeeva, Hao Shen, Peter Vollhardt.

S09
Joint X-Ray and Neutron Crystallography at the Protein Crystallography Station. Zoe Fisher, Andrey Kovalevsky, Marc Michael Blum, Marat Mustyakimov, Mary Jo Waltman, Paul Langan.

S10
Metal-Organometallic Frameworks. K. Travis Holman, Sayon A. Kumalah Robinson.

S11
Structural Determinants of Tobacco Vein Mottling Virus Protease Substrate Specificity. David Waugh, Ping Sun, Brian Austin, Jozsef Tozser.

S12
Structural Basis for Promoter -10 Element Recognition by the Bacterial RNA Polymerase Sigma-Subunit. Andrey Feklistov, Seth Darst.

S13
Rio1 Kinase: Structure-Based Inhibitor Design and Oligomeric State Characterization. Irene Kiburu, Nicole LaRonde-LeBlanc.

S14
Carbonic Anhydrase: Inhibitors and Activators. Mayank Aggarwal, Fabbio Pacchiano, Balendu Avvaru, Arthur Robbins, Claudiu Supuran, Robert McKenna.

# Posters-S

S15
Interactions of Toll-Like Receptors (TLR1 and TLR2) With a Heat-Labile Enterotoxin B Pentamer (LT-IIb-B5) Using SAXS and Crystal Structures of Surface Mutants of LT-IIb-B5. Vivian Cody, Jim Pace, Tom Grant, Joe Luft, Edward Snell, Terry Connell, Hesham Nawar, George Hajishengallis.

S16
Potential Model Complexes for Nickel Superoxide Dismutase. Tom Mwania, David Eichhorn.

S17
Hints for Refining Low-Resolution Protein X-Ray Structures. Vishal Koparde, Glen Kellogg, Neil Scarsdale.

S18
Alkali Metal-Coordination Cages for Selective Sulfate Binding and Separation. Arbin Rajbanshi, Arbin Rajbanshi, Bruce A. Moyer, Radu Custelcean.

S19
Structural Basis for 5'-Nucleotide Base-Specific Recognition of Guide RNA by Human AGO2. Filipp Frank.

S20
Wanted Defects and Distortions!. Melissa Menard, Gregory T. McCandless, Kandace R. Thomas, Julia Y. Chan.

S21
X-Ray Crystallography and Isothermal Titration Calorimetry Studies of the Salmonella Zinc Transporter ZntB. Qun Wan.

S22
SCrALS: Challenging Samples, Straightforward Solution - the Continuing Story. Allen Oliver, Jeanette Krause.

S23
Automating Low Volume Protein Crystallography Set-Ups Using Mosquito. Joby Jenkins, Ben Schenker, Rob Lewis, Chloe Carter.

S24
Crystal Structure of Get4/Get5 Complex and Its Interactions With Sgt2, Get3 and Ydj1. Chwan-Deng Hsiao, Yi-Wei Chang, Yuh-Ju Sun, Chung Wang.

S25
The Use of Co-Crystals for the Determination of Absolute Stereochemistry. Kevin Eccles, Rebecca Deasy, Laszlo Fabin, Anita Maguire, Simon Lawrence.

S26
X-Ray Structural Studies of Novel Dicyanomethylydene Chromophores. Joel Zazueta, Paul Tongwa, Alexandr Fonari, Ilya Kosilkin, Emily Hillenbrand, Marina Fonari, Larry Dalton, Tatiana Timofeeva.

S27
Diamond Hard-Wearing in Nuclear Reactor Core. Boris Udovic.

S28
Crystal Engineering the Covalent Bond. Leonard MacGillivray.

S29
Structural Characterization of An Unusual Heme Cofactor in Hydroxylamine Oxidoreductase. Peder Cedervall, Alan Hooper, Carrie Wilmot.

S30
Synthesis and Structural Characterisation of Pt(II) Complexes With Non- Covalent Interactions. Sara Fuertes, Simon K. Brayshaw, Mark W. Warren, Paul R. Raithby.

S31
Non Ambient Crystallographic Studies of Dithienylethene Optical Molecular Switches. Christopher Woodall, Paul Raithby, David Allan.

S34
Controlling the Negative Thermal Expansion and Compressibility of ScF3 Through Cation Substitution. Cody R. Morelock, Benjamin K. Gre, Angus P. Wilkinson.

S35
Crystal Structures of Histone and P53 Methyltransferase SmyD2 Reveal a Conformational Flexibility of the Autoinhibitory C-Terminal Domain. Yuanyuan Jiang, Nualpun Sirinupong, Joseph Brunzelle , Zhe Yang.

S36
Biochemical and Crystallographic Studies of the Type III Secretion Translocator Sipb and Its Chaperone Sica From *Salmonella enterica.* Amit Priyadarshi, Liang Tang.

S37
Structural Insights Into the Binding Mechanism of (R)- and (S)-Naproxen With Cyclooxygenase-2. Surajit Banerjee, Kelsey C. Duggan, Daniel J. Hermanson, Joel Muse, Jeffery J. Prusakiewicz, Jami L. Scheib, Bruce D. Carter, John A. Oates, Lawrence J. Marnett.

S38
Structural Insights Into the Autoinhibition and Posttranslational Activation of Histone Methyltransferase SmyD3. Nualpun Sirinupong, Nualpun Sirinupong, Joseph Brunzelle, Ernada Doko, Zhe Yang.

S39
G-Rob: a Flexible, Multitask 6-Axis Robotic-Arm Based Systems for Crystallography. Jean-Luc Ferrer, Xavier Vernede, Jacques Joly, Florian Bouis, Nathalie Larive, Pierre Mazel, Pierrick Rogues, Jean-Loup Rechatin, Yaser Heidari, Michel Pirocchi.

S41
Insights Into Phenyl Motion During the Racemization of Mandelate by Mandelate Racemase. Adam Lietzan, Elise Pellmann, Mitesh Nagar, Jennifer Bourque, Stephen Bearne, Martin St Maurice.

S42
C-H vs. N-H as H-Bond Donors in Cyano-Substituted Phenylhydrazones. William Ojala, Shakeyla Barber, Emily Rohkohl, Charles Ojala.

S43
Molecular Bases of Enantioselectivity of Haloalkane Dehalogenase DbjA. Yukari Sato, Zbynek Prokop, Jan Brezovsky, Ryo Natsume, Yuji Nagata, Jiri Damborsky, Toshiya Senda, Radka Chaloupkova.

S44
Comparison of the Molecular Structures of μ-oxo Iron(III) Porphyrin Malaria Pigment Model Compounds. Saifon Kohnhorst, Kenneth Haller.

S45
Water Dimers in the Structure of NiV2O6 2H2O. Aungkana Chatkon, Kenneth Haller.

S47
Disorder in the Dihydrate of a Derivative of Acyclovir. Montha Meepripruk, Kenneth Haller.

S48
Best Data Collection Strategies in Practice. Gleb Bourenkov, Alexander Popov.

S49
Relationship of Structure and Luminescence Property in Nanoporous Metal Phosphates and Phosphites. Sue-Lein Wang.

S50
Structural Characterization of Lead Hydroxyapatite. Oratai Saisa-ard, Kenneth J. Haller.

S51
Co2 Separation and Hydrogen Storage Properties of Copper and Silver Exchanged Zeolites for Clean Energy Applications. Matthew Hudson, Wendy L. Queen, Craig M. Brown, Dustin W. Fickel, Bharat Boppana, Raul F. Lobo.

S53
Structure and Properties of Hybrid O-Me2TTF Salts Containing Halide, Linear, Polyoxometalate and Cyanometalate Anions. Eric Reinheimer, Hanhua Zhao, Andrey Prosvirin, Codi Sanders, Marc Fourmigue, Kim Dunbar.

S54
Dispositions of the Rod-Like Solvates Cs2 and I2 in the Nanotubular-Like Packing of C70 Structures. Faye Bowles, Marilyn Olmstead, Alan Balch.

S55
The Role of Total Scattering and Multiscale Modeling in the Technological Development of Geopolymer Concrete. Claire White, John Provis, Neil Henson, Katharine Page, Thomas Proffen, Jannie van Deventer.

S56
Montmorillonite Modification by Cationic Surfactants. Ana Bianchi, M Fernandez, M Pantanetti, Raul Vina, Iris Torriani, Rosa M. Sanchez, Graciela Punte.

S57
Confocal Microscopy on the Beamline: Novel 3D Imaging and Sample Positioning. Imran Khan, Warren Zipfel, Rebecca Williams, Richard Gillian, Ulrich Englich.

S58
Structural Insights Into Substrate Specificity in Two Copper Amine Oxidases From *Hansenula polymorpha*. Valerie Klema, Cindy Chang, Bryan Johnson, Minae Mure, Judith Klinman, Carrie Wilmot.

S59
Insights Into the Lithiation of Nano-Sized alpha-Fe2O3: a Combined X-Ray Absorption Spectroscopy and Pair Distribution Function Study. Badri Shyam, Karena Chapman, Swati Pol, Robert Klingler, Mahalingam Balasubramanian, Steve Heald, Giselle Sandi-Tapia, George Srajer, Peter Chupas.

S60
Mail-In Crystallography: Convenient Use of the Canadian Macromolecular Crystallography Facility. Shaunivan Labiuk, James Gorin, Kathryn Janzen, Michel Fodje, Pawel Grochulski.

S61
X-Ray Study of Mono- and Di-Carbonyl-Bridged Tricyclic Heterocyclic Acceptors. Bhupinder Sandhu, Paul Tongwa, Yulia Getmanenko, Seth Marder, Tatiana Timofeeva.

S62
Differential Effects of Substrates and Substrate Analogues on the Conformational States of the Bacterial Cell Wall Biosynthetic Enzyme Mura. Jin-Yi Zhu, Yan Yang, Stephane Betzi, Ernst Schonbrunn.

S63
Status of Three Proposed MX Beamlines at NSLS-II. Dieter Schneider, Marc Allaire, Lonny Berman, Mark Chance, Wayne Hendrickson, Annie Heroux, Jean Jakoncic, Qun Liu, Lisa Miller, Allen Orville. Howard Robinson, Wuxian Shi, Alex Soares, Vivian Stojanoff, Deborah Stoner-Ma, Robert Sweet.

S64
Data Processing and Assessment of Quality in Time-Resolved Laue Diffraction of Excited Species of the Organometallic Complex Rh2(M-Pnp)2(Pnp)2Bph4. Anna Makal, Jason Benedict, Jaroslaw Kalinowski, Jesse Sokolow, Elzbieta Trzop, Philip Coppens.

S65
Effect of Supramolecular Structure on Molecular Structure in a Titanium(III) Oxalate Dimer: Ti2((-C2O4)(C2O4)2(H2O)6 2H2O. Orrasa In-Noi, Kenneth J. Haller.

S66
Synthesis of Metal-Porphyrin-Framework Structures. Michelle Everett, Claudia Rawn, David Keffer.

S67
Recent Bio-Science From the Center for Structural Molecular Biology at Oak Ridge. Volker Urban, William Heller, Kevin Weiss, Hugh O'Neill, Sai Venkatesh Pingali, Shuo Qian, Dean Myles.

S68
Design of New Magnesium Coordination Networks Using Solvents as Structure Directing Agents. Debasis Banerjee, Jeffrey Finkelstein, John B. Parise.

S69
High Temperature X-Ray Powder Diffraction Studies of Mayenite. Claudia Rawn, Sabina Ude, Andrew Payzant.

S70
Solutions to Local Structural Problems in Catalysis: Combining Infrared Spectroscopy and Pair-Distribution-Function Analysis. Kevin Beyer, Haiyan Zhao, Karena Chapman, Mark Newton, Peter Chupas.

S71
The SER-CAT Facility Upgrade: Current Status and Future Plans. John Chrzas, John Gonczy, James Fait, Zhongmin Jin, Zheng-Qing Fu, Roderick Salazar, John Rose, Bi-Cheng.

S72
X8 Prospector: Using In-House Screening to Help Improve Productivity During Synchrotron Trips. Matthew Benning.

S73
Imagine, a Quasi-Laue Single Crystal Neutron Diffractometer at the High Flux Isotope Reactor. Flora Meilleur, Parthapratim Munshi, Tibor Koritsanszky, Robert Blessing, Bryan Chakoumakos, Dean Myles.

S74
Complementary Technology to the Synchrotron. Pierre Le Magueres, Angela Criswell, Joseph Ferrara, Bret Simpson.

S75
The Structural Biology Center User Program at the Advanced Photon Source, Argonne National Laboratory. Stephan Ginell, Randy W. Alkire, Changsoo Chang, Marianne E. Cuff, Norma E.C. Duke, Youngchang Kim, Krzysztof Lazarski, Jack Lazarz, Mike Molitsky, Bogi Nocek. J. Osipiuk, S.O. Park, G. Rosenbaum, F.J. Rotella, K. Tan, R-G. Zhang, A. Joachimiak.

S76
Rapid Automated Processing of Data (RAPD) Software Package. Jonathan Schuermann, David Neau, Frank Murphy.

S77
Improvements in High Pressure Research Capabilities on Beamline 1222 at the Advanced Light Source. Jason Knight, Alastair MacDowell, Simon Clark, Howard Padmore, Selva Raju, Bin Chen, Jinyuan Yan, Lowell Miyagi, Jane Kanitpanyacharoen, Quentin Williams.

S78
Structure of CFA/I Fimbriae from Entorotoxigenic *Escherichia coli*, the Bacteria that Cause Diarrhea. Rui Bao, Esther Bullitt, Stephen J Savarino, Di Xia.

S79
A Novel High-throughput Approach for Purification and Reconstitution of Large Multiprotein Complexes. Filippo Pullara, Monica Calero, Qiangmin Zhang, Hilary Stevenson, Guillermo Calero.

## Monday Posters

M01
High Energy Resonant XRD and Differential Atomic Pair Distribution Function Studies of Complex Materials. Valeri Petkov, Sarvjit Shastri.

M02
Real Structure of TSSG Grown Large *Barium hexaferrite* Single Crystals Studied by White Beam X-Ray Transmission Topography. Kraeusslich Juergen, Ortrud Wehrhan, Sebastian Hoefer, Carsten Dubs, Peter Goernert.

M03
Structural Insights Into the Stabilizing Contributions of Chemically- Modified Nucleic Acids. Ella Czarina Juan, Satoru Shimizu, Xiao Ma, Taizo Kurose, Tsuyoshi Haraguchi, Takeshi Kurihara, Jiro Kondo, David Williams, Akira Matsuda, Akio Takenaka.

M04
Structure and Histone Binding Properties of the Vps75-Rtt109 Chaperone-Lysine Acetyltransferase Complex. Dan Su, Qi Hu, Hui Zhou, James R. Thompson, Zhiguo Zhang, Georges Mer.

M05
On the Systematic Scaling and Merging of Multiple Crystals in Macromolecular Crystallography General Framework and First Results. James Foadi, Gwyndaf Evans, Robin Owen, Danny Axford, Wes Armour, David Waterman, Yilmaz Alguel, Alex Cameron.

M06
Structures of Inhibitor and Substrate Complexes of Golgi alpha-Mannosidase II Reveal the Basis for Fragment-Based Anti-Cancer Compounds. David Rose, Douglas Kuntz, Niket Shah, B. Mario Pinto.

M07
Inhibition of Recombinant Maltase-Glucoamylase and Sucrase-Isomaltase by Novel Inhibitors. Kyra Jones, Lyann Sim, Sankar Mohan, Jayakanthan Kumarasamy, Hui Liu, Stephen Avery, Roberto Quezada-Calvillo, Buford L. Nichols, B. Mario Pinto, David R. Rose.

M08
Cloning and Expression of a Glycoside Hydrolase Family 31 Enzyme From *Bacteroides thetaiotaomicron*. Marcia Chaudet, David Rose.

M09
Structural Features of the Unusual Thiolase Olea That Facilitate Long-Chain Hydrocarbon Biosynthesis. Brandon Goblirsch, Janice Frias, Larry Wackett, Caroline Wilmot.

M10
Crystals From the Direct One-Pot Synthesis of Calix[4]Arenes With 1,3-Dibromopropane. Shimelis Hailu, Paul F. Hudrlik, Anne M. Hudrlik, Ray J. Butcher.

M11
Systematic Approach to Better Crystals. Qiang (James) Zhao, Qian(Frank)Wang, Tiantang Dong, Xinjun Liu, Xiaoshu Hou, Yuanna Zhai, Yujun Han, Huili Hou, Michelle Xia, Maxwell Wang.

M12
New Approaches to Time-Resolved Structural Studies of Macromolecules. Briony Yorke, Arwen Pearson, Mike Webb, Robin Owen.

M13
Hidden Phase Transitions and Transformation Mechanisms of Nat-Topology Zeolites in T-P(H2O) Space. Hsiu-Wen Wang, David L. Bish.

M14
Structural Insights Into Pseudouridine 5'-Phosphate Glycosidase. Siyu Huang, Steven Ealick.

M15
Structure of the CMP Hydrolase, MilB, Re-

veals Basis of Substrate Recognition and Catalysis. Megan Sikowitz, Steven Ealick.

M16
Structurally Similar But Functionally Different Zu5 Repeats in Human Erythrocyte Ankyrin. Mai Yasunaga, Jonathan Ipsaro, Alfonso Mondragon.

M17
Developing the Laue Method for Multicrystal Structure Determination. Doletha Szebenyi, Donald Bilderback, Ulrich Englich, Qingqiu Huang, Chae Un Kim, Irina Kriksunov, Mark Pfeifer, Detlef Smilgies.

M18
Structural Insights in to C Rotundicauda Serine Protease Inhibitor Domain- 1: Design and Development of a Potent Thrombin Inhibitor. Pankaj Kumar Giri, Jeak Ling Ding, Kunchithapadam Swaminathan, J. Sivaraman.

M19
A Paradigm for Glycan Acquisition by the Human Distal Gut Bacteroidetes: the Starch Utilization System (Sus) of Bacteroides Thetaiotaomicron. Nicole Koropatkin, Elizabeth Cameron, Eric Martens, Thomas Smith, Christopher Smith, Julie Biteen, Jeffrey Gordon.

M20
Correlating Changes in Structure and Function of Bacteroides Thetaiotaomicron Tetx2 to Fitness During Adaptation to Minocycline. Katarzyna Walkiewicz, Milya Davlieva, Christine Sun, Matthew Pena, Kelsey Lau, Yousif Shamoo.

M21
Structure-Function Relationships Study of the Glutathione-S-Transferase Superfamily in the Saprophytic Fungus Phanerochaete Chrysosporium. Claude Didierjean, Pascalita Prosper, Edgar Meux, Melanie Morel, Eric Gelhaye, Guillermo Mulliert, Frederique Favier.

M22
The Crystal Structure of 2-(3-Fluoro-5-(Pyridinium-3-Yl)Benzamido)-6-Methylpyridinium Dibromide. Mark Frisch, Santosh Kulkarni, Amy Hauck Newman, Jeffrey R. Deschamps.

M23
High-Flux Micro Beam Is Effective to Collect Diffraction Data From Tiny Macromolecular Crystals. Kunio Hirata, Yoshiaki Kawano, Koichi Hashimoto, Go Ueno, Takaaki Hikima, Hironori Murakami, Nobutaka Shimizu, Kazuya Hasegawa, Takashi Kumasaka, Masaki Yamamoto.

M24
Invariom Modeling of a Short Fragment of "DNA". Kevin Proepper, Julian Holstein, Birger Dittrich.

M25
The Crystal Structure of the Catalytic Domain of the Endosome-Associated Deubiquitinating Enzyme, Amsh. Christopher Davies, Lake Paul, Chittaranjan Das.

M26
Structure of Glpx Encoded Fructose 1,6 - Bisphosphatase From *M tuberculosis*. Hiten Gutka, Hiten Gutka, Cele Abad- Zapatero, Scott Franzblau, Farahnaz Movahedzadeh.

M27
Insights Into Cooperative Binding of TraM to oriT DNA From the Crystal Structure of the pED208 Plasmid TraM-sbmA Complex. Joyce Wong, Jun Lu, Ross Edwards, Laura Frost, Mark Glover.

M28
Structure of Human C8 Protein Provides Mechanistic Insight Into Membrane Pore Formation by Complement. Leslie Lovelace, Christopher L. Cooper, James M. Sodetz, Lukasz Lebioda.

M29
Structure Function Studies of Vaccinia Virus

Host-Range Protein C7L Reveal a Unique Beta Fold Structure. Brian Krumm, Yongchao Li, Xiangzhi Meng, Yan Xiang, Junpeng Deng.

M30
Detection of Microcrystals by Second Order Nonlinear Optical Imaging of Chiral Crystals (SONICC). David Kissick, Ellen Gualtieri, Mark Hunter, Petra Fromme, Vadim Cherezov, Robert Fischetti, Garth Simpson.

M31
High-Resolution Structures Reveal Halide Ion Binding to Optogenetic Chloride Sensors Constructed by Protein Engineering Automation. Weina Wang, Joshua Grimley, Lorena Beese, Homme Hellinga.

M32
Crystal Structure of PhoP From Mycobacterium tuberculosis. Shuishu Wang, Smita Menon.

M33
Diagnosing Secondary Structure Pathologies at Low Resolution. Christopher Williams, Jane Richardson, David Richardson.

M34
D-Periodic Molecular Structure of Type II Collagen *in situ* to its Native Tissue. Joseph Orgel, Olga Antipova.

M35
Structure, Function and Evolution of the Spo0B Phosphotransferase. Shraddha Thakkar, Vidya Harini Veldore, Reha Celikel, Kottayil I. Varughese.

M36
Interactions Between HypE and HypF Hydrogenase Maturation Factors. Svetlana Petkun, Rong Shi, Yonge Li, Jean Francois Trempe, Abdalin Asinas, Christine Munger, Miroslaw Cygler.

M37
Substrate and Product Complexes of Wild Type and Mutant *E. coli* QueD. Sue Roberts, Reid McCarty, Vahe Bandarian.

M38
Identification of Selective Enzyme Inhibitors by Small Molecule Fragment Library Screening. Alexander Pavlovsky, Geng Gao, Nina Potente, Ronald Viola.

M39
Human Udp-Xylose Synthase in Solution; Crystallographic Contacts Gone Wild. Samuel J Polizzi, Richard Walsh Jr., Zachary A. Wood.

M40
Crystal Structure of GroEL Chaperonin From *Chlorobium tepidum*. Changsoo Chang, Lance Bigelow, Norman Marshall, Brian Feldman, Gekleng Chhor, Youngchang Kim, Andrzej Joachimiak, Robert Jedrzejczak.

M41
A Detailed Catalytic Cycle for Human UDP-Glucose Dehydrogenase. Nicholas Sennett.

M42
Structure and Mechanism of Processing Alpha-Glucosidase I. Megan Barker, David Rose.

M43
Total Scattering at the Lujan Center. Katharine Page, Anna Llobet, Joan Siewenie.

M44
When Single Crystals Are Not Available - Opportunities for Solving Pharmaceutical Crystal Structures Using Powder X-Ray Diffraction. Hyunsoo Park, Qi Gao.

M45
11-ID-B: a Dedicated Instrument for X-ray Pair Distribution Function Measurements. Karena Chapman, Kevin Beyer, Peter Chupas.

M46
Neutron Single Crystal Diffraction From Experiment Planning to Analysis. Christina Hoffmann, Xiaoping Wang, Matthew Frost,

Janik Zikovky, Dennis Mikkelson, Ruth Mikkelson, Arthur Schultz, Peter Peterson.

M47
Structure of Unsolvated Chloronitrosylbis(Triphenylphosphine)Nickel. Kenneth Haller, Pinsa Boonkon.

M48
Development of a Dedicated Pair-Distribution-Function Beamline at the Advanced Photon Source: Scientific Drivers and Opportunities. Peter Chupas.

M49
The Crystal Structure of the P27 Component of Human Dynactin. Anna Kowalska, Meiying Zheng, Urszula Derewenda, Zygmunt S. Derewenda.

M50
1-BM: a Versatile Instrument for in situ X-Ray Diffraction Studies. Gregory Halder, John Okasinski.

M51
SSAD_DB: a Database of Structures Solved by Sulfur SAD Phasing and Related Experimental Parameters. John Rose, Hua Zhang, Manfred Weiss, Bi-Cheng Wang.

M52
Hidden Symmetries in Disordered Matter. Miguel Castro-Colin, Christian Gutt, Peter Wochner, Tina Autenrieth, Thomas Demmer, Vladimir Bugaev, Alejandro Diaz Ortiz, Federico Zontone, Gerhard Gruebel, Helmut Dosch.

M53
Structural Studies of Carbonic Anhydrase Inhibitor Complexes: Towards Developing Isoform Specificity. Shyamasri Biswas, Mayank Aggarwal, Alfonso Maresca, Arthur H. Robbins, Claudiu T. Supuran, Robert McKenna.

M54
The Photo-Excited State of the Organometalic Complex [Rh2(μ-PNP)2(PNP)2] 2Bph4 by Single-Pulse Pump-Probe Laue Diffraction. Elzbieta Trzop, Jason J. Benedict, Jaroslaw Kalinowski, Anna Makal, Jesse Sokolow, Philip Coppens.

M55
Structure of Dimethylsulfoniopropionate-Dependent Demethylase. David Schuller, Chris Reisch, Mary Moran, William Whitman, William Lanzilotta.

M56
Quantum Mechanical DFT Analysis of Copper Dynamic Behavior in Doped Zinc and Cadmium-Histidine Crystals. Michael Colaneri, Kristin Kirschbaum, Jacqueline Vitali.

M57
New Single Crystal Diffraction and SAXS Instrumentation With Bright and Low Maintenance Sources. Sergio Rodrigues, Ronan Mahe, Olivier Pacaud, Peter Hoghoj.

M58
Removing the Mystery From Mystery Density in X-Ray Crystallography With Single-Crystal Spectroscopy. Allen Orville, Deborah Stoner-Ma, PXRR Group.

M59
'Rational' Stochastic Crystallization Screen Design for High-Throughput Protein Crystallography. Jared Liu, Li-Wei Hung.

M60
First-Principles Calculations of Ultrahigh-Field Solid State NMR Lineshapes: Benchmarking Calculations and Experimental Measurements. Gary Enright, Peter Pallister, Igor Moudrakovski, John Ripmeester.

M61
X-Ray and Neutron Crystallographic Structure-Based Mechanism of Archaeal Inorganic Pyrophophatase From *Thermococcus thioreducins*. Joseph D. Ng, Ronny C. Hughes, Leighton Coates, Matthew P. Blakeley, Stephen J. Tomanicek, Edward J. Meehan, Juan M. Garcia-Ruiz.

M62
CheckMyMetal (CMM): Validation of Metal Binding Sites in Protein Structures. Heping Zheng, Mahendra Chordia, David Cooper, Maksymilian Chruszcz, Wladek Minor.

M63
Automated Tools for Finding a Crystal Sample and Mapping Its Quality. Ruslan Sanishvili, Mark Hilgart, Sergey Stepanov, Michael Becker, Venugopalan Nagarajan, Sudhirbabu Pothineni, Craig Ogata, Janet Smith, Robert Fischetti.

M64
Pseudoracemic Crystallization of a Small Protein Containing Pentafluorophenylalanine in Its Hydrophobic Core. David Mortenson, Kenneth Satyshur, Katrina Forest, Samuel Gellman.

M65
Towards the Structure of Haemophilus Influenzae Kdo Kinase. Tinoush Moulaei, Alexander Wlodawer.

M66
A Continuously Variable Piezoelectric Beam Collimator. Simon Morton, Jeff Dickert, Paul Adams.

M67
Ultrafast Structural Phase Transition of FeRh. Donald Walko, Eric Landahl, Jin Wang.

M68
We Present a PDF Analysis of Different Species Intercalated in Nanoporous Materials the First Study is for a Series of Thiol-Functionalized Mesoporous Silicas With Different Mercaptopropyl Content and Hg Loading, Materials That Are Effective Trapping Age. Mouath Shatnawi, Simon Billinge, Thomas Pinnavia, Jame Dye, Emily McKimmy, Gianluca Paglia.

M69
Crystallization and Preliminary X-Ray Analysis of the Transcription Factor Complex of NKX25 and TBX5 With Target DNA. Lagnajeet Pradhan, Sunil Kumar Gopal, Sandhya Ramesh, Hyun-Joo Nam Nam.

M70
Selectively Synthesis Trans-Azo Dimer by Photoreaction and Identification of Triplet Azo Intermediate in Solid State. Qian Li, Jeanette Krause , Anna Gudmundsdottir.

M71
Cloning, Purification, Crystallization and Preliminary X-ray Analysis of the Catalytic Domain of Human Receptor-like Protein Tyrosine Phosphatase gamma in Three Different Crystal Forms. Kevin Kish, Patricia McDonnell, Valentina Goldfarb, William Metzler, David Langley, James Bryson, Susan Kiefer, Brian Carpenter, Walter Kostich, Steven Sheriff.

M72
Recent Developments in the SuperNova Dual Source Micro-focus Diffractometer. Zoltan Gal, Alexandra Griffin, Oliver Presly.

M73
Guided Ligand Replacement (GLR). Herbert Klei, Matt Pokross, Shana Posy, Thomas Terwilliger, Paul Adams, Nigel Moriarty.

M74
Crystal Structures of PKG IŒ≤ (92-227) with cGMP and cAMP Reveal the Molecular Details of Cyclic-nucleotide Binding. Gilbert Huang, Jeong Joo Kim, Darren Casteel, Taek Hun Kwon, Ronnie Ren, Peter Zwart, Jeffrey Headd, Nicholas Brown, Dar-Chone Chow, Choel Kim.

M75
Crystal Structure Analysis of Nectin and Nectin Like Molecule Family. Mamoru Suzuki, Hirotaka Narita, Atsushi Nakagawa.

## Tuesday Posters

T01
Using SAXS and WAXS Methods for Nanomaterial Analysis. Akhilesh Tripathi, Aya Takase.

T02
A Structure Prediction Method for Remote Homologs Using Supersecondary-Structure Building Blocks and Basic NMR Data. Andras Fiser, Vilas Menon, Andras Fiser.

T03
WAXS Studies of the Structural Diversity of Protein Ensembles. Lee Makowski.

T04
Macrosnap: Software for Rapidly Comparing, Clustering and Visualizing 3-D Protein Structures Mined From the PDB. Chris Gilmore, Stuart Mackay, Gordon Barr, Wei Dong, Adrian Lapthorn.

T05
Protein Structure Determination by Exhaustive Search of the RCSB Protein Data Bank Derived Databases. Ian Stokes-Rees, Piotr Sliz.

T06
Crystal Structures of P63 DNA Binding Domain in Complexes With 10- and 22-Basepair Response Elements: Modes of Tetramerization and DNA Superhelix Conformations. Chen Chen, Osnat Herzberg.

T07
Identification of the DNA Repair Active Site of Topoisomerase V by Structural and Functional Studies. Rakhi Rajan, Rajendra Rajendra Prasad, Bhupesh Taneja, Samuel H Wilson, Alfonso Mondragon.

T08
Utilizing a Supramolecular Protecting Group Strategy to Facilitate [2+2] Cycloaddition Reactions in the Organic Solid State. Ryan Groeneman, Elizabeth Elacqua, Poonam Kaushik, Leonard MacGillivray.

T09
X-Chip: An Integrated Platform for High-Throughput Protein Crystallization and Off-The-Chip X-Ray Diffraction Data Collection. Nickolay Chirgadze, Gera KIsselman, Wei Qiu, Vladimir Romanov, Christine Thompson, Robert Lam, Kevin Battaile, Emil Pai.

T10
Structural Studies on Therapeutic Antibodies for Prion Diseases. Michael James, Pravas Baral, Mridula Swayampakula, Barbara Wieland, Rahman Muhammad, M. Polymenidou, Adriano Aguzzi, Nat Kav.

T11
Ancestral Protein Sheds Light on Steroid Receptor Cross-Pharmacology. Eric Ortlund, Jeffrey Kohn.

T12
Structural, Computational, and Biophysical Studies of Monocarbam-Siderophore Conjugate, Mc-1. Seungil Han, Richard Zaniewski, Eric Marr, Brian Lacey, Andrew Tomaras, Arterm Evdokimov, J. Richard Miller, Xidong Feng, Kieran Geoghegan, Veerabahu Shanmugasundaram.

T13
Facilities for Macromolecular Crystallography at BESSY II - Berlin. Uwe Mueller, Martin Bommer, Nora Darowski, Ronald Forster, Michael Steffien, Michael Krug, Karthik Paithankar, Sandra Puhringer, Manfred Weiss.

T14
The UvrA UvrB DNA Damage Sensor: Structure and Mechanism. David Jeruzalmi, Danaya Pakotiprapha, Martin Samuels, Koning Shen, Johnny Hu.

T15
Using a Conformationally-Dependent Stereochemical Library Improves Crystallographic Refinement of Proteins. Dale Tronrud, Donald Berkholz, P. Andrew Karplus.

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Utilization of Single Crystal X-Ray Studies of Process Relevant Pharmaceutical Crystal Forms to Support QbD. Michael Galella, John DiMarco, Raymond Scaringe, Carolyn Pommier, Jack Gougoutas.

T17
Structural Studies of K11-Linked Ubiquitin. Christine Yu, Ken Dong, Marissa Matsumoto, Lilian Phu, Bob Kelley, Don Kirkpatrick, Vishva Dixit, Sarah Hymowitz.

T18
MoleCoolQt - a Molecule Viewer for Charge-Density Research. Christian Huebschle, Birger Dittrich.

T19
Design of New Cocrystal Forms of Apixaban - Preparation of Isostructural Solid Forms by Replacing Multiple Water Molecules With Single Coformers. Marta Dabros, V. Rosso, M. Liu, R Schlam, M.F. Malley, R.P. Scaringe.

T20
Relibase+ : Generating Knowledge From Both Public and Proprietary Structural Data. Colin Groom.

T21
Remote Access to Spring-8 Px Beamlines. Go Ueno, Kazuya Hasegawa, Takaaki Hikima, Hironori Murakami, Yukito Furukawa, Takashi Kumasaka, Masaki Yamamoto.

T22
Characterization of the Influence of the Water Miscible Ionic Liquid 1-Butyl-3-Methylimidazolium Chloride With Model Proteins. William Heller, Gary Baker, Hugh O'Neill, Qiu Zhang.

T23
Hydrogen Bonding in the Crystal Structures of Hydantoins and Related Molecules. Carl H. Schwalbe, Aurora J. Cruz-Cabeza.

T24
Crystallization and X-Ray Crystal Structures of Sulfapyridine and Sulfapyridine Cocrystallized With Dioxane, Tetrahydrofuran, and Piperidine. Cheryl Stevens, Jamal Pratt, Janna Hutchinson.

T25
Crystal Structures of Human Interferon Lambda in Complex With its Extracellular Receptor at 21Å Resolution. Zachary Miknis, Eugenia Magracheva, Wei Lei, Alexander Zdanov, Sergei Kotenko, Alexander Wlodawer.

T26
The Protein Data Bank at 40 - No Time for a Mid-Life Crisis. Jasmine Young, Shuchismita Dutta, Zukang Feng, Aleksandras Gutmanas, Miriam Hirshberg, Takanori Matsuura, Steve Madding, Tom Oldfield, Ardan Patwardhan, Martha Quesada. Sanchayita Sen, Jawahar Swaminathan, Eldon Ulrich, Sameer Velankar, Marina Zhuravleva, John Westbrook, Gerard Kleywegt, Haruki Nakamura, Ardan Patwardhan, John Markley, Helen Berman.

T27
Hydroxyl Orientations in Cellobiose and Other Polyhydroxy Compounds - Modeling Vs Experiment. Alfred French, Gabor Csonka.

T28
Macromolecular Data Collection and Processing Using Crysalispro and the Supernova. Tadeusz Skarzynski.

T29
Detection of Crystal Radiation Damage Through Real Time Data Collection. Zhongmin Jin, John Chrzas, John Rose, B.C. Wang.

T30
Twinning on Cooling: Self-Inflicted Wounds. FrankR. Fronczek .

T31
SAD Phasing Using Iodide Ions in a High-Throughput Structural Genomics Environment. Thomas Edwards, Jan Abendroth, Bart Staker, Peter Myler, Lance Stewart.

T32
CCP4 62 - 32 Years in the Making . Ronan Keegan, Charles Ballard, Eugene Krissinel, Martyn Winn.

T33
Autoprocess: An Automated Strategy Calculation and Data Processing Pipeline for Macromolecular Crystallography Experiments. Michel Fodje, Kathryn Janzen, Pawel Grochulski, Shaunivan Labiuk, James Gorin.

T34
The HB2A High Resolution Powder Diffractometer at the High Flux Isotope Reactor. Clarina de la Cruz.

T35
Biophysical Analysis of Conformational Changes in Adeno-Associated Viruses Under Endosomal Ph Conditions. Balasubramanian Venkatakrishnan, Shuo Qian, Barry Byrne, Nicholas Muzyczka, Mavis Agbandje-McKenna, Robert McKenna.

T36
Removing a Persistent, Publication-Preventing Difference Peak From a Single- Crystal Structure Analysis. Larry Falvello, Sonia Martinez-Salvador, Babil Menjon.

T37
Home Beam Line: Concurrent Data Collection, Processing, and Structure Solution With Hkl-3000R. Michael Murray.

T38
Unfurling of the F2 Ferm Domain of Merlin Tumor Suppressor. Sollepura Yogesha, Andrew Sharff, Marco Giovannini, Gerard Bricogne, Tina Izard.

T39
Binding of alpha-Thrombin to Platelet Glycoprotein Ib alpha Sulfotyrosines Through a Two-Site Mechanism Involving Exosite I and Exosite II. Kottayil Varughese, Alessandro Zarpellon, Reha Celikel, James Roberts, Richard McClintock, Loredana Mendolicchio, Kevin Moore, Zaverio Ruggeri.

T40
A Laboratory Information Management System for Macromolecular Crystallography Experiments at the Canadian Light Source. Kathryn Janzen, Michel Fodje, Pawel Grochulski, Shaunivan Labiuk, James Gorin.

T41
What's in a Drop? Correlating Observations and Outcomes to Guide Macromolecular Crystallization Experiments. Edward H. Snell, Jennifer R. Wolfley, Joseph R. Luft.

T42
High-Throughput BioSAXS: Disposable Tip Pipetting and Quick-Change Capillary Flow Cells. Richard Gillilan, Magda Moller, Soren Nielsen.

T43
Crystal Structure of Yeast Jac1 Co-Chaperone. Jerzy Osipiuk, Lance Bigelow, Rory Mulligan, Brian Feldmann, Szymon Ciesielski, Jaroslaw Marszalek, ElizabethA. Craig, Andrzej Joachimiak.

T44
Sg-Lims: Coping With the Complexities of Htp Cloning, Protein Purification, and Protein Crystallization. Gyorgy Babnigg, Hao An, Patrick Eschenfeldt, Andrzej Joachimiak.

T45
Crystal Structures of a Therapeutic Single Chain Antibody in Complex With Two Drugs of Abuse and Their Psychologically-Active Metabolites. Reha Celikel, Eric Peterson, Michael Owens, Kottayil Varughese.

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Improvements to On-Axis Visualization (OAV) at GM/CA CAT Beamlines at the APS. Nagarajan Venugopalan, Shenglan Xu, Steve Corcoran, Sudhir Pothineni, Oleg Makarov, Sergey Stepanov, Janet Smith, Robert Fischetti.

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Chemical Crystallography for Undergraduate Research: Unexpected and Fruitful Results. Gary Nichol, Stephanie Hurst, Edward Rajaseelan.

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The Joint Center for Structural Genomics: Tools and Resources for the Community. Marc-Andre Elsliger, Ashley M. Deacon, Adam Godzik, Scott A. Lesley, John Wooley, Kurt Wuthrich, Ian A. Wilson.

T49
A Salvage Protein Purification Approach in Mcsg High-Throughput Pipeline. Ruiying Wu, Hui Li, Gyorgy Babnigg, Youngchang Kim , Andrzej Joachimiak.

T50
C-Hal...Hal Nonbonded Intermolecular Interactions in Molecular Crystals. Raymond Davis.

T51
The Structure of a Hexahistidine-Tagged Form of Augmenter of Liver Regeneration Reveals a Novel [Cd2Cl4O6] Cluster That Aids in Crystal Packing. M. Gary Newton, Quentin Florence, Chia-Kuei Wu, Jeffrey Habel, James Swindell II, Bi-Cheng Wang, John Rose.

T52
Understanding Time, Length, and Energy Scales in Radiation Damage to Protein Crystals. Matthew Warkentin, Jesse Hopkins, Ryan Badaeu, Robert Thorne.

T53
Cooling Rate- and Temperature-Dependence of a Highly Mobile "Flap" Covering the Active Site of Urease. Robert Thorne, Matthew Warkentin, Andrew Karplus.

T55
SONICC Miniaturization for Direct Implementation Onto Synchrotron Beamlines for Protein Crystal Detection and Automated Centering. Jeremy Madden, David Kissick, Garth Simpson.

T56
Sample Environments at ORNL Neutron Facilities. Lisa DeBeer-Schmitt, John Christenson, Rebecca Mills, Saad Elorfi, Enrique Robles, Brian Plante, Randy McPhearson, Lou Santodonato.

T57
Online Size-Exclusion Chromatography for Solution X-Ray Scattering Studies on Challenging Protein Systems. Lester Carter, Hiro Tsuruta.

T58
A Novel Approach to Automatic Scoring of Protein Drop Images Using UV Fluorescence. Max Petersen, Mandel Mickley, Chris Boarman, Giles Mullen.

T59
Indexing and Integration of Small Molecule Laue Diffraction Data. Jaroslaw Kalinowski, Anna Makal.

T60
Functional Classification and Structural Characterization of Immune Regulatory Proteins. Rotem Rubinstein, Udupi Ramagopal, Andras Fiser, Steven Almo.

T61
BIOSAXS-1000 - a New Tool for Gaining Structural Insight When Crystallographic Methods Aren't Enough. Angela Criswell.

T62
Three-Dimensional Models for All Binary and Ternary Protein Complexes of the Cyanobacterial Kaiabc Circadian Oscillator and the Clock Output Kinase Sasa. Rekha Pattanayek, Dewight Williams, Tetsuya Mori, Gian Rossi, Steven Weigand, Carl Johnson, Phoebe Stewart, Martin Egli.

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A High-Performance Small Angle X-Ray Scat-

tering Instrument - Rigaku Nanomax tm. Lixin Fan, Mike Degen, Licai Jiang, Scott Bendle, Paul Pennartz, Nick Grupido.

T64
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T65
Structural Characterization of the Role of Nep1, a Psuedouridine N1-Specific Methyltransferase, in Ribosome Biogenesis. Nicole LaRonde-LeBlanc, Seth Thomas, Christopher Keller, Agnieszka Syzk, Joseph Cannon.

T66
Applications of Pairwise Comparison and Classification of the Ligand Binding Sites in Protein Three-Dimensional Structures. Stephane Richard, Moriaud Fabrice, Olivia Doppelt-Azeroual, Stephane Richard, Francois Delfaud.

T67
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T68
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Remote Access at LS-CAT. David Smith, Keith Brister, Max Brister.

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Deployment of a Robotic Protein Crystal Harvester in a High Throughput Crystallography Environment. Bernhard Rupp, Bob Viola, Jace Walsh, Alex Melka, Wesley Womack, Sean Murphy, Alan Riboldi-Tunnicliffe, Marc A. Elsliger, Marc C. Deller, Ian A. Wilson.

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Structure of the Catalytic Chain of M. jannaschii Aspartate Transcarbamoylase in a Hexagonal Crystal Form. Jacqueline Vitali, Aditya Singh, Nermina Covic, Alexei Soares, Michael Colaneri.

T72
Crystal Structure of ER-resident Protein Disulfide Reductase ERdj5. Mamoru Suzuki, Masatoshi Hagiwara, Kenichi Maegawa, Jun Hoseki, Kazuhiro Nagata, Kenji Inaba.

T73
Crystal Structure of ER-resident Protein Disulfide Reductase ERdj5. Mamoru Suzuki, Masatoshi Hagiwara, Kenichi Maegawa, Jun Hoseki, Kazuhiro Nagata, Kenji Inaba.

T74
NE-CAT Crystallography Beamlines for Challenging Structural Biology Research. Kanagalaghatta Rajashankar, Steven Ealick, Malcolm Capel, Surajit Banerjee, Frank Murphy, Igor Kouriniv, David Neau, Kay Perry, Jonathan Schuermann, Narayanasami Sukumar.

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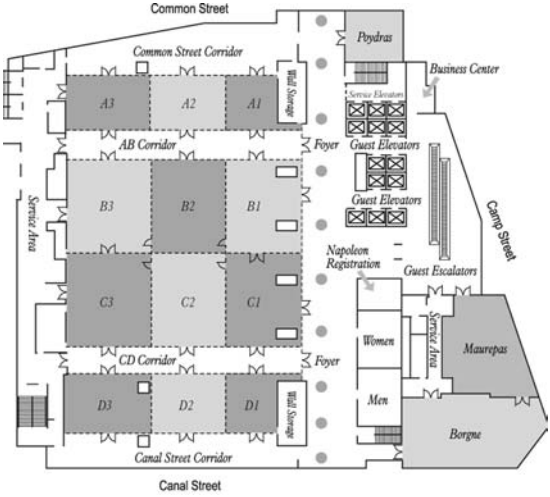
## 3rd Floor

**ACA Registration Desk, session rooms, exhibit & poster hall**

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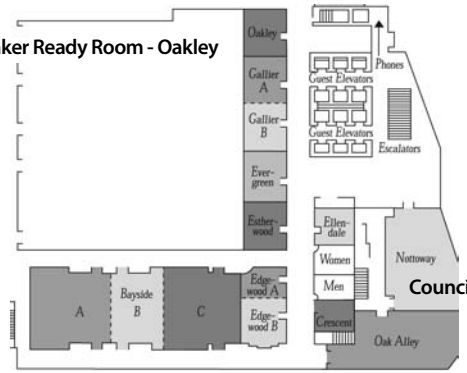


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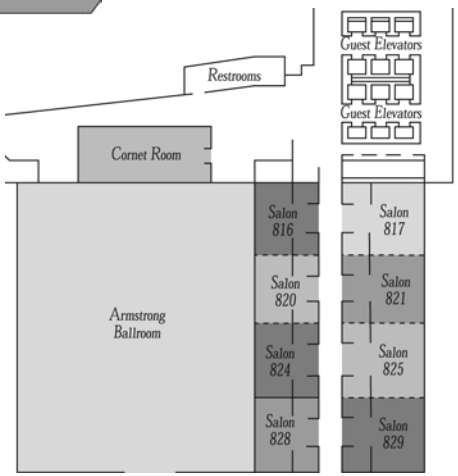

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# NAPOLEON BALLROOM, SHERATON NEW ORLEANS

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