Boston 2012

American Crystallographic Association

Annual Meeting

July 28 - August 1, 2012
Boston, MA

Program

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July 28 - August 1, 2012, Boston, MA

Program Chairs: Bruce Foxman and Bruce Noll

Local Chair: Peter Müller **Poster Chair: Ilia Guzei**

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Small Molecules ..... Shao-Liang Zheng
Synchrotron Radiation ..... Craig Ogata
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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, ACA RefleXions, the association's 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 Scientific Interest Groups (SIGs) 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 SIG 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.

Boston logo design by Christina Landolt and Peter Müller

WK.01 Refmac and Coot

Paul Emsley, Garib Murshudov, Presiding
Harbor I

9:00am - Morning

Introduction to refinement
Roberto Steiner
- Bonds and angles etc.
- How to define them (mmCIF files)
- How to acquire and review restraints for known ligands

Refinement at low resolution
Garib Murshudov
- Working with NCS
- Working with Jelly bodies

Refinement II
- Twinning
- Sharpening

Ligands for chemistry: Few case studies
Roberto Steiner

Ligands: Jligand and link restraints
Garib Murshudov

Model building in coot
Paul Emsley
- Rotamer optimisation
- Ramachandran Refinement
- Finding and fixing bumps (Molprobity tools)
- Hands-on: Keybindings, scripting
- Placing ligands

Afternoon

- Tutorials (or demos) on refinement at low resolution ligand and link design
- Coot in general

Instructors:
Paul Emsley, paul.emsley@bioch.ox.ac.uk
Garib Murshudov, garib@mrc-lmb.cam.ac.uk
Roberto Steiner

WK.02 Structure Refinement and Disorder Modeling with OLEX2

Ilia Guzei, Presiding
Harbor II

Funding for this workshop provided by OlexSys Limited

OLEX2 is an actively developed graphics program for structural solution and refinement. The workshop aims to introduce a number of advanced structure refinement features available in OLEX2 to a wide audience. The workshop will introduce a typical OLEX2 workflow followed by several in-depth examples of how non-routine structures may be refined. Particular attention will be paid to refinement of disordered structures and what advantages OLEX2 offers in handling them. The participants will be immediately given an opportunity to test these procedures and apply their new skills on provided problem structures. Three OLEX2 experts will be present. The participants will be shown how OLEX2 takes advantage of underutilized but extremely useful features of SHELX and an alternative to the popular SQUEEZE routine of PLATON. A special presentation on the molecular graphics features of OLEX2 is also planned. The benefit to the crystallographic community is an improved ability to model many types of disordered structures in a facile fashion.

08:30-08:45 Ilia Guzei - Introduction / outline

08:45-09:15 Horst Puschmann - Workflow in OLEX2

09:15-9:30 File Editing/Refinement options

9:30-10:00 An example of refining the atomic occupancy factors

10:00-10:30 Coffee break

10:30-11:00 A detailed example of a structure with positional disorder

11:00-11:30 A detailed example of a structure with disorder and tricky H atoms assignment

11:30-12:00 A detailed example of changing space group (P1 to P-1)

12:00-1:00 Lunch (provided)

01:00-02:00 Oleg Dolomanov Use of idealized molecular geometries for modeling misbehaved entities (FRAG/FEND)

02:00-02:30 Use of solvent masks to account for diffusely diffracting species

02:30-03:30 Oleg Dolomanov Molecular graphics with OLEX2 and PovRay (from a single molecule to packing diagrams)

03:30-04:00 Coffee break

04:00-04:45 Horst Puschmann Preparation of a publication-ready CIF files and accompanying materials.

04:45-06:00 Discussion of the users' examples, Q and A

6:00-6:3 Group discussion of results / progress / survey

Instructors:

Oleg Dolomanov, OlexSys Limited, oleg@olexsys.org

Horst Puschmann, OlexSys Limited, horst@olexsys.org

Ilia Guzei, University of Wisconsin-Madison, iguzei@chem.wisc.edu

WK.03 Modeling and Refinement of Nanoparticle Structures from Diffraction Data

Katharine Page, Thomas Proffen, Reinhard Neder Lewis

Nanomaterials are becoming of increasing importance as complex, functional materials and without a doubt, this trend will continue. Whereas we have a well-developed set of tools to structurally characterize crystalline materials from single crystal and powder diffraction data, tools to extract the same amount of structural information from nanomaterials are just emerging. Along with new tools comes the challenge of making them available to the wider community and more importantly providing the training needed to enable young crystallographers to enter this field.

Filling this need is the aim of this workshop proposal centered around the modeling and refinement programs PDFgui and DISCUS. What is unique and new in this workshop is the focus on nanoparticles (particles with a diameter less than 100 nanometers) based on total scattering x-ray and/or neutron data. This is the first hands-on workshop that will cover approaches based on a bulk-like model (PDFgui) as well as the simulation of discreet particles (DISCUS).

PDFgui (www.diffpy.org) is freely available and runs on Windows, MAC and Unix based platforms. The program enables refinement of a structural model to the experimental atomic pair distribution function (PDF). The program is usually used to model disordered bulk materials. However, the use of an envelope function for finite particles allows refining PDFs from spherical nanomaterials. A recent example of this technique applied to BaTiO3 nanoparticles can be found in "Probing Local Dipoles and Ligand Structure in BaTiO3 Nanoparticles" by Page et al., Chemistry of Materials 22, 4386 (2010) - DOI: 10.1021/cm100440p.

DISCUS (discus.sourceforge.net) employs an alternate strategy and allows one to create the actual finite particle and refine appropriate

model parameters using an evolutionary algorithm. This is the approach of choice in cases where a bulk type model fails, e.g. interactions with organic capping molecules, core-shell architectures, or anisotropic shapes. Details were published recently in "Building and refining complete nanoparticle structures with total scattering data" by Page et al.,J.Appl.Cryst.,44,327 (2011) - DOI: 10.1107/S0021889811001968

08:00-09:00 Welcome and introduction to nanoparticle analysis. T. Proffen

09:00-10:00 Modeling of the spherical nanoparticle PDF and introduction to PDFgui and the hands-on example. K. Page

10:00-10:30 Coffee Break

10:30-12:00 - PDFgui hands-on example. T. Proffen / K. Page

12:00-01:00 Lunch (on your own)

01:00-02:00 - Creating /refinement of discreet nanoparticle models and introduction to DISCUS and the hands-on example. T. Proffen

02:00-03:00 - DISCUS hands-on (Part I). T. Proffen / K. Page

03:00-03:30 Coffee Break

03:30-05:00 DISCUS hands-on (Part II). T. Proffen / K. Page

Instructors:
Katherine Page, page@lanl.gov
Thomas Proffen, tproffen@ornl.gov

WK.04 Crystallography - World of Wonders

Cora Lind, Claudia Rawn, Presiding
Burroughs

08:30-09:15 Demonstration: Smart-X2S
Bruce Noll, Bruker

9:15-10:15 Materials Discovery Camp Part I
Claudia Rawn, ORNL, UT Knoxville
Making Structures with Lego, Ping-Pong Balls and Yarn

10:15-10:30 Coffee Break

10:30-11:30 Materials Discovery Camp Part II Claudia Rawn, ORNL, UT Knoxville
Making Structures with Lego, Ping-Pong Balls and Yarn

11:30-12:15 Diffraction Basics
Cora Lind, U. Toledo

12:15-01:00 Lunch (provided)

1:00-1:15 Structure solution of aspirin
Bruce Noll, Bruker

1:15-1:45 Remotely enabled instruments - a new paradigm for teaching crystallographic science
Katherine Kantardjieff, CSU San Marcos

1:45-2:45 Understanding Everyday Materials using X-ray Powder Diffraction
Jim Kaduk, Illinois Inst of Technology, Chicago

2:45-3:00 Coffee Break

3:00-4:00 Tackling Some Difficult Concepts in High School and College Chemistry, using the Cambridge Structural Database, Colin Groom

4:00-4:45 Getting the Most Out of the Protein Data Bank, David Goodsell, Scripps Research Institute

SATURDAY, JULY 28

4:45-5:30 Biomolecule structures for the classroom

Instructors:
Cora Lind, cora.lind@utoledo.edu
David Goodsell, goodsell@scripps.edu
Katherine Kantardjieff, kkantard@csusm.edu
Jim Kaduk, kaduk@polycrystallography.com
Bruce Noll, bruce.noll@gmail.com
Colin Groom, secretary@ccdc.cam.ac.uk
Claudia Rawn, crawn@utk.edu

Saturday Evening Activities

Student and First Time Attendee Meeting Orientation

5:30pm **Lewis**

Faye Bowles, Presiding

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.

SP.01 Innovations in Undergraduate Education

6:30pm **Harbor II**

Bruce Foxman & David Rose, Presiding

A lecture by Eric Mazur, Harvard University

Opening Reception, Exhibit Show and Presidential Welcome

7:30pm **Galleria Hall**

Must have meeting name badge for entry

Registration Desk	07:30am	Galleria Foyer
Speaker Ready Room	07:30am	Griffin
Council Meeting Room	07:30am	Carlton
Exhibit Show	10:00am	Galleria Hall
Rigaku Users Luncheon (invitation only. pick up ticket at Rigaku booth)	12:00pm	Stone

Canadian Division Meeting	12:00-12:30pm	Lewis
General Interest Meeting	12:00-12:30pm	Burroughs
Synchrotron Rad SIG Meeting	12:00-12:30pm	Harbor II
BioMac SIG Meeting	1:00-1:30pm	Harbor III
SAS SIG Meeting	1:00-1:30pm	Harbor I
Poster Session S	5:30-7:30pm	Galleria Hall
YSSIG Mixer (ticket required)	8:00pm	Harbor I & II

AW.01 Buerger Award Presentation and Lecture - John Spence

George Phillips, Presiding
Harbor I

08:00-09:00am **AW.01**
Fast Molecular Imaging with an X-ray Laser. John C.H. Spence

01.01 Protein Structure Initiative: More Tools for the Home Lab

Ward Smith, Presiding
Harbor III

09:00-09:20am **01.01.01**
PSI Structural Biology Knowledgebase: New Ways to Enable Your Research. Margaret Gabanyi, John Westbrook, Yi-Ping Tao, Raship Shah, David Micallef, William McLaughlin, Torsten Schwede, Paul Adams, Wladek Minor, Helen Berman.

09:20-09:40am **01.01.02**
SAD Phasing Using Iodide Ions in a High-Throughput Structural Genomics Environment. Thomas Edwards, Jan Abendroth, Bart Staker, Peter Myler, Lance Stewart.

09:40-10:00am **01.01.03**
Robust Experimentation Tools for Real or Virtual Trips to Synchrotron Beamlines. Ruslan Sanishvili, Craig Ogata, Venugopalan Nagarajan, Michael Becker, Sergey Stepanov, Mark Hilgart, S. Xu, Sudhirbabu Potineni, D. Yoder, Oleg Makarov, Janet Smith, Robert Fischetti.

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

10:30-10:50am **01.01.04**
The PSI:Biology-Materials Repository: A Resource for Protein Expression Plasmids. Catherine Cormier, Jin Park, Jason Steel, Michael Fiacco, Preston Hunter, Jason Kramer, Joshua LaBaer.

10:50-11:10am **01.01.05**
Rational Engineering of Improved Protein Crystallization. John Hunt, Victor Naumov, Helen, Lena Street, Sergey Vorobiev, Alexandre Kuzin, Farhad Forouhar, Thomas Acton, Rong Xiao, Montelione Gaetano.

11:10-11:30am **01.01.06**
Improving Chances of Successful Structure Determination. Adam Godzik, Lukasz Jaroszewski.

11:30-11:45am **01.01.07**
When to do a MAD Experiment? Surajit Banerjee, Kanagalaghatta Rajashankar.

11:45-12:00pm **01.01.08**
New Versatile Cryoprotection Technique using Water-soluble Polymer Glue with Humidity control. Seiki Baba, Takeshi Hoshino, Takashi Kumasaka.

01.02 Structural Approaches to Enzyme Mechanisms

Karen Allen, Presiding
Harbor III

01:30-02:00pm **01.02.01**
A Methyl Hand-off Between B Vitamins is Caught in the Act. Cathy Drennan, Yan Kung, Nozomi Ando, Tzanko Doukov, Leah Blasiak, Gunes Bender, Javier Seravalli, Stephen Ragsdale.

02:00-02:15pm **01.02.02**
Structural Basis for Recognition of 5'-phosphotyrosine Adduct by TDP2. Hideki Aihara, Ke Shi, Kayo Kurahashi.

02:15-02:30pm **01.02.03**
The Structural Basis of PP1 Regulation and Specificity. Rebecca Page, Wolfgang Peti.

SUNDAY, JULY 29

02:30-03:00pm **01.02.04**
What Looks Like a Duck, but Doesn't Quack? Structure and Function in Family V of the Acetoacetate Decarboxylase-Like Superfamily. Nicholas Silvaggi, Lisa Mueller.

03:00-03:30pm Coffee Break

03:30-04:00pm **01.02.05**
Human Mitochondrial PheRS in Dynamics: Crystal Structure Manifests Transition From "Closed" to Active "Open" State Upon Substrate tRNAPhe Binding. Mark Safro, Liron Klipcan, Nina Moor, Igal Finarov.

04:00-04:15pm **01.02.06**
Capturing Reaction Intermediates in *bacteriophytochrome* by Temperature-Scan Cryocrystallography. Xiaojing Yang, Zhong Ren, Jane Kuk, Keith Moffat.

04:15-04:30pm **01.02.07**
Conformational Leveraging in the Allosteric Response of Human UDP-glucose Dehydrogenase. Zachary A. Wood, Gregory Custer, Nicholas Sennet, Renuka Kadirvelraj.

04:30-05:00pm **01.02.08**
The Structure of an Integral Membrane Ion-Pumping Pyrophosphatase Suggests a Third Solution for Coupling Phosphoanhydride Bond Hydrolysis to Vectorial Ion Transport. Adiran Goldman, Juho Kellosalo, Tommi Kajander, Konstantin Kogan.

03.01 General Interest I

Allen Oliver, Presiding
Lewis

01:30-02:00pm **03.01.01**
Forensic Crystallography (I): The Ligand That Was Not There. Edwin Pozharski, Christian X Weichenberger, Bernhard Rupp.

02:00-02:30pm **03.01.02**
Spherical Eggs, Bananas, and Pancakes - Use and Misuse of B Factors and Thermal Ellipsoids. Ethan Merritt.

02:30-03:00pm **03.01.03**
Forensic Crystallography (II): The F-calc Files. Bernhard Rupp.

03:00-03:30pm Coffee Break

03:30-04:00pm **03.01.04**
The Use of CMOS Active Pixel Sensors for X-ray Crystallographic Analysis. Charles Campana, Bruce Noll, Michael Ruf, Roger Durst.

04:00-04:30pm **03.01.05**
Is A "Benchtop" Diffractometer Suitable For Research? Lee Daniels.

04:30-05:00pm **03.01.06**
Post Corrections in Area Detector Data Reduction. Mathias Meyer.

09.01 Functional Nanomaterials

Tad Koga, Kevin Yager, Presiding
Lewis

09:00-09:30am **09.01.01**
Facile Route to Vertically Aligned High Aspect Ratio Block Copolymer Films via Dynamic Zone Annealing. Gurpreet Singh, Manish Kulkarni, Kevin Yager, Detlef Smilgies, David Bucknall, Alamgir Karim.

09:30-10:00am **09.01.02**
Directing Order and Orientation in Organic Photovoltaic Thin Films. Kevin Yager, Htay Hlaing, John Allen, Danvers Johnston, Theanne Schiros, Ben Ocko, Charles Black.

10:00-10:30am Coffee Break

10:30-11:00am **09.01.03**
In-situ and Real-time GISAXS Studies of Processing NanoStructured Organic Thin Films. Detlef Smilgies.

11:00-11:30am **09.01.04**
Piezoelectric Properties of Nonpolar Block Copolymers. Volker Urban, Markus Ruppel, Christian W. Pester, Jimmy Mays, Alexander Böker.

11:30-12:00pm **09.01.05**
Revealing the Formation Process of Polymer Adsorption from the Melt onto Impenetrable Surfaces. Tad Koga, Peter Gin, Naisheng Jiang, Zexi Han, Fen Chen, Chen Liang, Maya Endoh.

13.01 Emerging Sources: Theory and Practice I

Marius Schmidt, Yun-Xing Wang, Presiding
Burroughs

09:00-09:20am **13.01.01**
Accurate High-throughput Macromolecular Structures in Solution by X-ray Scattering (SAXS): Leverging Databases with Rapid Data Collection from Next Generation Light Sources. John Tainer, Greg Hura, Robert Rambo, Michal Hammel.

09:20-09:40am **13.01.02**
Ultrafast Time-resolved X-ray Studies of Protein Dynamics. Friedrich Schotte, Philip Anfinrud, Hyun Sun Cho, Naranbaatar Dashdorj, Mikio Kataoka.

10:00-10:30am Coffee Break

10:30-10:50am **13.01.04**
Structure of Viruses from Scattering of Radiation from X-Ray Free-Electron Laser (XFEL). Dilano Saldin, Hin-Cheuck Poon, Miraj Uddin, Peter Schwander, Haiguang Liu, John Spence.

10:50-11:10am **13.01.05**
The Development of Femtosecond Relativistic Electron Diffraction. Pietro Musumeci, Renkai Li.

11:10-11:30am **13.01.06**
Serial Femtosecond Crystallography at the LCLS. Uwe Weierstall, R.B. Doak, J.C.H. Spence, P. Fromme, H.N. Chapman, S. Boutet.

11:30-11:50am **13.01.07**
X-ray Science at an FEL Pump-probe Instrument. Henrik Till, Lemke, Diling Zhu, Matthieu Chollet, Marco Cammarata, David Mark Fritz.

11:50-12:10pm **13.01.08**
Crystallography at a Hard X-ray Free Electron Laser. Marc Messerschmidt, Sebastien Boutet, Garth Williams.

13.02 Magnetic Materials

Ashfia Huq, Presiding
Harbor II

Funding for this session provided, in part, by Avanti Polar Lipids, Inc.

09:00-09:30am **13.02.01**
Magnetic Neutron Scattering in Oxygen-deficient Perovskites. John Greedan, Farshid Ramezanipour, Lachlan Cranswick, Donaberger Ronald, Ovidiu Garlea.

09:30-10:00am **13.02.02**
Spin Correlations in the Extended Kagome Systems $RBaCo_4O_7$. Dmitry Khalyavin.

10:00-10:30am Coffee Break

10:30-11:00am **13.02.03**
The Structural and Magnetic Ordering in Copper-based Delafossite Oxides. Ovidiu Garlea.

11:00-11:20am **13.02.04**
High Pressure as a Probe of Magneto-Structural Correlation in Molecular Magnets. Simon Parsons.

11:20-11:40am **13.02.05**
Effects of Random Exchange in Ferromagnetic Copper Chloride Chains. Susan Herringer, Mark Turnbull, Christopher Landee, Jordi Ribas-Arino, Merce Deumal, Juan Novoa.

11:40-12:00pm **13.02.06**
Investigation of Single Crystal Holmium Titanate Grown under Changing Conditions by the Optical Floating Zone Method. Timothy Munsie, Graeme Luke, Hanna Dabkowska.

13.03 Fibril-Forming Pathological Peptides: Prions, Amyloids, and "Friends"

Olga Antipova, Joseph Orgel, Presiding
Harbor II

01:30-01:45pm **13.03.01**
Prospective on Recent Structural Biology Advances in the Fields of Amyloid and Peptide based Brain Disease Research. Joseph Orgel.

01:45-02:15pm **13.03.02**
Insights from Fiber Diffraction into the Structures of Alzheimer's Aβ and Other Amyloids and Prions. Gerald Stubbs, Wen Bian, Tracy Fetterly, Amy Kendall, Michele McDonald, Jan Stoehr, William Wan.

02:15-02:40pm **13.03.03**
Crystal Structures of Rabbit Fabs Specific for Amyloid Oligomers and Fibrils. Hiromi Arai, Charles Glabe, Hartmut Luecke.

02:40-03:05pm **13.03.04**
Small-angle Neutron Scattering to Investigate Huntington Protein Aggregation in Huntington's Disease. Christopher Stanley, Tatiana Perevozchikova, Penney McWilliams-Koeppen, Valerie Berthelier.

03:05-03:30pm Coffee Break

03:30-03:50pm **13.03.05**
Structural Polymorphism of the Fungal Prion HET-s(218-289): Implications on the Generic Amyloid Structure. William Wan, Holger Wille, Jan Stöhr, Wen Bian, Michele McDonald, Gerald Stubbs.

03:50-04:10pm **13.03.06**
Structure and Inhibition of Mitogen-activated Protein Kinase Kinase 4 (MEK4): a Prostate cancer Pro-invasion Protein. Sankar Narayan Krishna, Chi-Hao Luan, George Minasov, Ludmilla Shuvalova, Rebecca Farmer, Antoinette Nibbs, Xiaoke Huang, Karl Scheidt, Wayne Anderson, Raymond Bergan.

04:10-04:30pm **13.03.07**
Structural Studies of Human Neonatal Fc Receptor. Mohammed Taha, Uta Bussmeyer, E. Sally Ward, Hyun-Joo Nam.

04:30-04:50pm **13.03.08**
Pseudo-Origin in Crystals of Anti-HIV-1 Neutralizing Antibody PG16. Robyn Stanfield, Robert Pejchal, Ian Wilson.

04:50-05:10pm **13.03.09**
Crystal Structure of the Nucleoprotein in the Infectious Salmon Anemia Virus. Wenjie Zheng, Yizhi Tao.

05:10-05:30pm **13.03.10**
Eliminating GI Drug Toxicity by Selectively Inhibiting a Symbiotic Bacterial Enzyme. Adam Roberts, Bret D. Wallace, Amanda LoGuidice, Makani Dollinger, Urs A. Boelsterli, Sridhar Mani, Matthew R. Redinbo.

13.04 Emerging Sources: Theory and Practice II

Volker Urban, Lin Yang, Presiding
Burroughs

01:30-02:00pm **13.04.01**
The Biological Small Angle Scattering/Diffraction Facility Beamline 4-2 at SSRL. Thomas M. Weiss, Tsutomu Matsui, Lester Carter, Ping Liu, Hiro Tsuruta.

02:00-02:30pm **13.04.02**
The Biological Small-Angle Scattering Instrument (Bio-SANS) at the Center for Structural Molecular Biology (CSMB) at Oak Ridge National Laboratory. Sai Venkatesh Pingali, Shuo Qian, Volker Urban, Kevin Weiss, Hugh O'Neill, Qiu Zhang, William Heller, Paul Langan.

02:30-03:00pm **13.04.03**
Upgraded BM29 Beamline for SAXS on Proteins in Solution at the ESRF. Petra Pernot, Adam Round, Pascal Theveneau, Werner Schmid, Mario Lentini, John Surr, Alexander Gobbo, Julien Huet, Florent Cipriani, Sean McSweeney.

03:00-03:30pm Coffee Break

03:30-04:00pm **13.04.04**
The EQ-SANS Instrument at the Spallation Neutron Source at Oak Ridge National Laboratory. William Heller, Changwoo Do, Christopher Stanley, Carrie Gao.

04:00-04:30pm **13.04.05**
X-ray Scattering for Life Sciences at NSLS-II: Preliminary Design of the LiX Beamline. Lin Yang.

04:30-05:00pm **13.04.06**
The New Very Small-Angle Neutron Scattering (VSANS) Diffractometer at NIST. John Barker, Charles Glinka, James Moyer, Nick Maliszewskyj.

TR.01 Transactions: Transformations and Structural Oddities in Molecular Crystals: In Honor of Bruce M. Foxman

G. Diaz de Delgado, M. Hickey, K. Wheeler, Presiding
Harbir I

Funding for this session provided, in part, by Alkermes, Inc., Bruker AXS, Inc., Crystal Growth & Design, Crystal Logic, Inc., and Rigaku Americas, Corp.

09:00-09:20am **TR.01.01**
Z'>1 Structures. Just a Nuisance or Something More Interesting? David Watkin, Richard Cooper, Anna Collins.

09:20-09:40am **TR.01.02**
Geometry and Reactivity in Crystalline Solids Formed by Transition Metal Citrate Cubanes. Larry R. Falvello, Elena Forcen-Vazquez.

09:40-10:00am **TR.01.03**
Molecular Flip and Photodimerization in the Solid-State. Menahem Kaftory, Thekku Veedu Sreevidya, Deng-Ke Cao, Mark Botoshansky.

10:00-10:30am Coffee Break

10:30-10:50am **TR.01.04**
A Clathrate Uncertainty Principle. Roger Bishop, Jiabin Gao, Djamal Djaidi, Mohan Bhadbhade.

10:50-11:10am **TR.01.05**
Synthesis and Transformations of New Iridium-Gold and Osmium-Gold Carbonyl Cluster Complexes. Richard Adams, Qiang Zhang, Xinzheng Yang.

11:10-11:30am **TR.01.06**
Learning from Outliers. Carolyn P. Brock.

11:30-11:50am **TR.01.07**
Hydrogen-bonded Zeolite-like Frameworks and Functional Materials. Michael Ward, Yuzhou Liu, Chunhua Hu, Airon Soegiarto.

11:50-01:30pm Lunch Break

01:30-01:50pm **TR.01.08**
Sulfonamidecinnamic Acids: Well-behaved Supramolecular Assemblies and Desymmetrized Single-Crystal Photodimerization Reactions. Kraig Wheeler.

01:50-02:10pm **TR.01.09**
Dynamic Photocrystallography: From Chemical Reactions to Short-lived Reactive Species. Philip Coppens.

02:10-02:30pm **TR.01.10**
Profound Effects of Crystal Symmetry on Physical Properties. Arnold Rheingold.

02:30-02:50pm **TR.01.11**
Twisted Crystals. Bart Kahr, Alexander Shtukenberg, Xiaoyan Cui, Ankit Gujral.

02:50-03:30pm Coffee Break

03:30-03:50pm **TR.01.12**
Engineering Reactions in Crystalline Solids by Taking Advantage of Reactive Intermediates. Miguel Garcia-Garibay, Saori Shiraki, Denisse de Loera.

03:50-04:10pm **TR.01.13**
Enantiotropic Serendipity: Using DSC to Assist in the Data Acquisition of Otherwise Routine Single Crystal Diffraction Experiments. Victor Young, Wesley Henderson, Michael Carney.

04:10-04:30pm **TR.01.14**
P•••I-R X-Bonding, Polymorphism, Mechanochemistry and WYSIWYG. William Pennington, Hadi Arman, Adam Siegfried, Dorota Abramovitch, Timothy Hanks.

04:30-04:50pm **TR.01.15**
Some Personal Recollections of Structural Oddities in Molecular Crystals. Joel Bernstein.

2012 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	Eugene Chun, The Scripps Research Inst.	13.20.05
Fiber Diffraction	Simon Goodson, Cardiff Univ.	13.11.03
General Interest	Karim Sutton, Univ. of Oxford	03.02.04
Industrial	Shraddha Thakkar, Univ. of Arkansas	13.22.06
Neutron Scattering	Elena Aksel, Univ. of Florida	13.13.01
Powder Diffraction	Andrey Yakovenko, Texas A&M Univ.	13.19.04
Small Angle Scattering	Allan Pang, Queen Mary Univ of London	09.05.07
Synchrotron Radiation	Christopher Dettmar, Purdue Univ.	13.12.05
Young Scientists	Joseph Liberman, Univ. of Rochester	12.01.09

Registration Desk ..... 07:30am ..... Galleria Foyer
Speaker Ready Room ..... 07:30am ..... Griffin
Council Meeting Room ..... 07:30am ..... Carlton
Exhibit Show ..... 10:00am ..... Galleria Hal
Agilent User Luncheon ..... 12:00pm ..... Otis
(by invitation only. secure ticket at Agilent booth)
Bruker Luncheon
(by invitation only. secure ticket at Bruker booth)
Fiber Diffraction SIG Meeting .... 12:00-12:30pm .. Harbor I

Service & Small Molecules SIGs
Joint Meeting ..... 12:00-12:30pm ..... Harbor III
Industrial SIG Meeting ..... 12:00-12:30pm ..... Harbor II
IUCr publBiodemo/lunch ..... 12:15pm ..... Webster
(by invitation only. secure a ticket at IUCr booth)
Neutron/Materials/Powder SIGS
Joint Meeting ..... 1:00-1:30pm ..... Harbor I
Young Scientists SIG Meeting ..... 1:00-1:30pm ..... Lewis
Poster Session M ..... 5:30-7:30pm ..... Galleria Hall

AW.02 Warren Award Presentation and Lecture - Paul Fenter

George Phillips, Presiding
Harbor I

08:00-09:00am **AW.02.01**
Imaging Structures and Processes at Solid-Liquid Interfaces with X-rays. Paul Fenter.

01.03 Structural Enzymology — Biology

Cynthia Stauffacher, Zachary Wood, Presiding
Harbor III

01:30-01:55pm **01.03.01**
Ultrafast Time-Resolved SAXS/WAXS Studies of Proteins in Solution. Philip Anfinrud, Hyun Sun Cho, Friedrich Schotte, Naranbaatar Dashdorj, John Kyndt.

01:55-02:20pm **01.03.02**
Elucidation of Intermediates in Cooperative Ligand Binding by Time-resolved Crystallography. William Royer, Zhong Ren, Vukica Srajer.

02:20-02:45pm **01.03.03**
Allosteric Competitive Inactivation of Hematopoietic CSF-1 Signaling by the Viral Decoy Receptor BARF1. Savvas Savvides, Jonathan Elegheert, Nathalie Bracke, Philippe Pouliot, Irina Gutsche, Alexander Shkumatov, Nicolas Tarbouriech, Wim Burmeister, Dmitri Svergun, Bjorn Vergauwen.

02:45-03:10pm **01.03.04**
Structural Basis of Toxicity and Immunity in Contact-Dependent Growth Inhibition (CDI) Systems. Celia Goulding, Robert Morse, Elias Gerrick, Angelina Iniguez, Keil Nikolakakis, Christopher Hayes.

03:10-03:30pm Coffee Break

03:30-03:50pm **01.03.05**
Inner Workings of the UvrA•UvrB DNA Damage Sensor during Bacterial Nucleotide Excision Repair. David Jerualmi, Danaya Pakotiprapha, Martin Samuels, Koning Shen, Johnny Hu.

03:50-04:10pm **01.03.06**
New Insights into Base Excision Repair of Alkylated DNA. Brandt Eichman, Suraj Adhikary, Emily Rubinson.

04:10-04:30pm **01.03.07**
The Structural Basis of DNA-packaging Initiation by the Bacteriophage Sf6 Terminase Small Subunit: a DNA-Spooling Device. Liang Tang, Haiyan Zhao, Yvonne Kamau, Theodore Christensen.

04:30-04:50pm **01.03.08**
A New Look at Glycogen Biogenesis - Conformational Plasticity of Glycogenin and its Maltosaccharide Substrate During Catalysis. D. Sean Froese, Apirat Chaikuad, Georgina Berridge, Frank von Delft, Udo Oppermann, Wyatt Yue.

04:50-05:10pm **01.03.09**
Locating Hydrogen Atoms in Enzymes Using Neutron Protein Crystallography. Flora Meilleur, Parthapratim Munshi, Tibor Koritsanszky, Robert Blessing, Bryan C. Chakoumakos, Dean A. Myles.

09.02 Macromolecular Science with Scattering Methods

Angela Criswell, Xiaobing Zuo, Presiding
Lewis

Funding for this session provided, in part, by Rigaku Americas Corp.

09:00-09:30am **09.02.01**
SAXS and FRET Produce Divergent Views of the Unfolded States at Low Denaturant Concentrations. Tobin Sosnick, James Hinshaw, Karl Freed.

09:30-09:50am **09.02.02**
Small Angle Scattering (SAS) Combined with Crystallography and Computation: Defining Accurate Structure of DNA Repair Machinery. Michal Hammel, Greg Hura, Robert Rambo, Scott Classen, David Schriemer, Susan Lees-Miller, John Tainer.

09:50-10:10am **09.02.03**
How the HIV Virus Selects its Own MRNA for Export: The Topology of the HIV- 1 Rev Response Element, a Molecular Beacon For Specificity and Cooperativity of Rev Binding. Xianyang Fang.

10:10-10:30am Coffee Break

10:30-11:00am **09.02.04**
RNA folding and ATP-dependent Chaperone Proteins Monitored by SAXS. Rick Russell, Inga Jarmoskaite, Anna Mallam, Pilar Tijerina, Mark Del Campo, Soenke Seifert, Liang Guo.

11:00-11:20am **09.02.05**
Unraveling the Conformational Switching of Riboswitch RNAs in Solution using SAXS and NMR. T. Kwaku Dayie.

11:20-11:40am **09.02.06**
Short SAXS Data Collection Times on Various Protein Standards using a Home X-ray Source and the BioSAXS-1000. Mark Del Campo, Angela Criswell, Katsunari Sasaki.

11:40-12:00pm **09.02.07**
Probing Early Events in Protein Folding by Interfacing Microfluidic Microsecond Mixing with Small-Angle X-Ray Scattering Detection at the BioCAT Beamline 18ID. Rita Graceffa, Raul Barrea, Sagar V. Kathuria, R. Paul Nobrega, C. Robert Matthews, Liang Guo, Osman Bilsel, Tom Irving.

13.05 Emerging Sources: Theory and Practice III

Keith Moffat, Presiding
Burroughs

09:00-09:30am **13.05.01**
Third and Fourth Generation Synchrotron Sources and Time-resolved Crystallography. Timothy Graber, Robert W. Henning, Irina Koshelev, Vukica Srajer, Zhong Ren, Keith Moffat.

09:30-10:00am **13.05.02**
Crystallographic Observation of Photodissociation at Sub-X-ray-Bunch Time Resolution. Zhong Ren, Vukica Srajer, Timothy Graber, Robert Henning, Irina Koshelev, Keith Moffat, William Royer Jr.

10:00-10:30am Coffee Break

10:30-11:00am **13.05.03**
Photoisomerisation Quantum Yield and Nonlinear Cross Sections with Femtosecond Excitation of the Photoactive Yellow Protein for Pump-probe Protein Diffraction. Jasper van Thor.

11:00-11:30am **13.05.04**
The Micro-beam Beamline at SPring-8 Opens a New Field of Protein Micro-crystallography. Masaki Yamamoto, Kunio Hirata, Yoshiaki Kawano, Koichi Hashimoto, Go Ueno, Takaaki Hikima, Hironori Murakami, Takashi Kumasaka.

11:30-12:00pm **13.05.05**
Structures of Biological Molecules in Superfluid Helium Droplets: Electron Diffraction.

Wei Kong, Jie Zhang, Lei Chen, William Freund.

13.06 Materials For a Sustainable Future I

G. Halder, A. Yakovenko, S.V. Pingali, Presiding
Harbor II

Funding for this session provided, in part, by Argonne Natonal Lab and Poly Crystallography, Inc.

09:00-09:05am Opening remarks

09:05-09:30am **13.06.01**
Single Crystal Structural Characterization of Porous Flexible MOFs for Carbon Capture Applications. Winnie Wong-Ng, Jeffrey Culp, Yu-Sheng Chen, Peter Zavalij, Jeffrey Deschamps.

09:30-09:55am **13.06.02**
Porous Materials with Pre-Designed Single-Molecule Traps for CO_2 capture. Hong-Cai Zhou.

09:55-10:30am Coffee Break

10:30-10:55am **13.06.03**
Uranium-Bearing Hybrid Materials: Speciation, Spectroscopy and Structural Systematics. Christopher Cahill.

10:55-11:15am **13.06.04**
Trapping Guests Within a Nanoporous Metal-organic Framework Through Pressure-Induced Amorphization. Karena Chapman, Dorina Sava, Tina Nenoff, Gregory Halder, Peter Chupas.

11:15-11:40am **13.06.05**
Crystalline Porous Covalent Hydrazone Frameworks. Fernando Uribe-Romo, Omar Yaghi.

11:40-12:00pm **13.06.06**
Mechanism of CO_2 Sorption and Interaction in a Highly Selective Nanoporous Solid. Debasis Banerjee, Anna Plonka, William Woerner, Zhijuan Zhang, Nour Nijem, Yves J. Chabal, Jing Li, John B. Parise.

12:00-01:30pm Lunch Break

01:30-01:55pm **13.06.07**
Modifying Native Crystalline Polysaccharide Ultrastructure Can Improve Its Chemical and Biological Processability to Fuels, Chemicals and Materials. Shishir Chundawat.

01:55-02:20pm **13.06.08**
Development of Biohybrid Photoconversion Systems Based on Plant Light Harvesting Complex II. Hugh O'Neill, Mateus Cardoso, Xiang Yu, Qiu Zhang, William Heller, Kunlun Hong, Volker Urban.

02:20-02:40pm **13.06.09**
Neutron Diffraction Studies of Mixed CO_2 - CH_4 Gas Hydrates. Michelle Everett, Claudia Rawn, Ashfia Huq, Bryan Chakoumakos, Tommy Phelps.

02:40-03:00pm **13.06.10**
Dye-Sensitized Solar Cells: Quantitative Structure-Property Relationships (QSPR) that Rationalize the Function of their Light Harvesting Dyes. Jacqueline Cole.

03:00-03:30pm Coffee Break

03:30-03:55pm **13.06.11**
Reaction Mechanism Studies in Li-ion Batteries: a Multipronged Approach. Natasha Chernova.

03:55-04:20pm **13.06.12**
Spatial Heterogeneity of Reactions in Battery Electrodes. Olaf Borkiewicz, Kamila Wiaderek, Karena Chapman, Peter Chupas.

04:20-04:45pm **13.06.13**
Defects and Disorder in High Performance Li-Ion Cathode Materials. Craig Bridges, Dong Wook Shin, Katharine Harrison, Arumugam Manthiram, Ashfia Huq, Mariappan Paranthaman.

13.07 Past Reflections and Future Directions: 100 Years of Diffraction and the 25th Anniversary of the Service Crystallography SIG

Louise Dawe, Curtis Haltiwanger, Presiding
Harbor III

09:00-09:20am **13.07.01**
100 Years of Structure Determination. Jenny Glusker.

09:20-09:40am **13.07.02**
Evolution of Small Molecule Crystallographic Instrumentation in North America. Susan Byram, Charles Campana, Daniel Frankel.

09:40-10:00am **13.07.03**
History of the Establishment and Development of X-Ray Analysis Methods in Russia - The USSR. Ivan Fedorchuk, Nikolai Fedorchuk, Victor Prikhodski.

10:00-10:30am Coffee Break

10:30-10:50am **13.07.04**
But Who Will Know What a Glide Plane Is? A Sobering Look Forward in Crystallography. Brian Toby.

10:50-11:10am **13.07.05**
A Unique Solution to Everyday Challenges: MAX3D. Hilary Jenkins, James Britten, Weiguang Guan.

11:10-11:30am **13.07.06**
Enabling all Scientists to Utilize Crystallography. Paul Swepston.

11:30-11:50am **13.07.07**
A Fistful of Photons. Christine M. Beavers, Simon J. Teat.

11:50-12:10pm **13.07.08**
Using Partial Observations, Partial Models and Partial Residuals in Least Squares Refinement. A.David Rae.

13.08 Exciting Structures

Eric Armstrong, Graeme Conn, Presiding
Harbor I

09:00-09:20am **13.08.01**
Crystal Structure of a Protein-mediated RNA Supercoil. Jason Stagno, Buyong Ma, Jess Li, Amanda Altieri, R. Andrew Byrd, Xinhua Ji.

09:20-09:40am **13.08.02**
Role of Structural Asymmetry in Signal Propagation Within a Response Regulator DNA Complex. Dinesh Yernool, Anoop Narayanan, Shivesh Kumar, Amanda Evrard, Lake Paul.

09:40-10:00am **13.08.03**
The First Structure of a Modified-Nucleotide DNA Aptamer in Complex With a Protein Target. Douglas Davies, Amy Gelinas, Chi Zhang, John Rohloff, Jeffery Carter, Daniel O'Connell, Sheela Waugh, Steven Wolk, Wesley Mayfield, Alex Burgin.

10:00-10:30am Coffee Break

10:30-10:45am **13.08.04**
Architecture of the Transport Channel of the Nuclear Pore Complex. Sozanne R Solmaz, Radha Chauhan, Gunter Blobel, Ivo Melcak.

10:45-11:00am **13.08.05**
Structural Insight into the Ion-Exchange Mechanism of the Sodium/Calcium Exchanger. Hua Li, Jun Liao, Weizong Zeng, David Sauer, Ricardo Belmares, Youxing Jiang.

11:00-11:20am **13.08.06**
Structural Basis for Flagellin Recognition by the TLR5 Immune Receptor. Sung-il Yoon, Oleg Kurnasov, Venkatesh Natarajan, Minsun Hong, Andrei Gudkov, Andrei Osterman, Ian Wilson.

11:20-11:40am **13.08.07**
Recognition of Glycolipids by Type I Versus Type II NKT Cells. Dirk Zajonc, Enrico Girardi, Igor Maricic, Jing Wang, Vipin Kumar, Esther Yu.

11:40-12:00pm **13.08.08**
Human Folate Receptor Structures Reveal Conformational States for Endocytic Trafficking of Folates and Folate-Targeted Therapeutics. Charles Dann III, Ardian Wibowo, Kristen Reeder, Joshua Carter, Wuyi Meng, Faming Zhang, Manohar Ratnam.

13.09 Protein and Small Molecule Crystallography at Undergraduate Institutions: Research, Pedagogy and Professional Development

Roger Rowlett, Kraig Wheeler, Presiding
Lewis

01:30-02:00pm **13.09.01**
Crystallography in the Undergraduate Setting: From Diffractometer Acquisition to Publishing Structures in Collaboration with Undergraduates. Joseph Tanski.

02:00-02:30pm **13.09.02**
A Research One University Reaching Out to Undergraduate Institutions. Carla Slebodnick.

02:30-03:00pm **13.09.03**
Protein X-ray Crystallography at a Predominantly Undergraduate Institution: Challenges and Practice of Building a Productive Laboratory. Roger Rowlett.

03:00-03:30pm Coffee Break

03:30-04:00pm **13.09.04**
Proteins, Powders and Small Molecules - Multidisciplinary Uses of X-ray Diffraction at an Undergraduate Institution. Douglas Juers.

04:00-04:30am **13.09.05**
Single Crystal and Powder X-ray Diffraction in an Undergraduate Research Laboratory. Alexander Norquist.

04:30-05:00pm **13.09.06**
Funding Strategies for Small-Molecule Single-Crystal X-ray Diffractometers at PUIs. Kraig Wheeler.

13.10 Radiation Damage

Stephan Ginell, Ana Gonzalez, Presiding
Harbor I

01:30-02:00pm **13.10.01**
Flirting with Radiation Damage: How Much Exposure is Too Much? James Holton.

02:00-02:30pm **13.10.02**
Radiation Damage in Macromolecular Crystallography: Practical Considerations. Elspeth Garman.

02:30-03:00pm **13.10.03**
Time-dependent Global Radiation Damage: Can it be Outrun? Matthew Warkentin, Ryan Badeau, Jesse Hopkins, Anne Mulichak, Lisa Keefe, Robert Thorne.

03:00-03:30pm Coffee Break

03:30-04:00pm **13.10.04**
Measurement of Mitigation of X-ray Radiation Damage in Macromolecular Crystallography by Sub-micron Line Focus Beam. Zou Finfrock, Edward Stern, Randy Alkire, Yizhak Yacoby, Kenneth Evans-Lutterodt, Aaron Stein, Norma Duke, Joshua Kas, Andrzej Joachimiak.

04:00-04:30pm **13.10.05**
Burning Crystals. Sandor Brockhauser, Olof Svensson, Ricardo Leal, Alexander Popov, Andrew McCarthy.

04:30-05:00pm **13.10.06**
A Novel Statistic for Radiation Damage Analysis. Graeme Winter.

13.11 Flesh and Blood: Intact and *in situ* Connective Tissue Diffraction Studies of Animals, Plants and Insect Bodies

Olga Antipova, Joseph Orgel, Presiding
Burroughs

01:30-01:50pm **13.11.01**
Fiber Diffraction of Collagen: A Historical Perspective. Barbara Brodsky.

01:50-02:15pm **13.11.02**
Collagen type II fibrillar Structure and its interactions with biglycan. Olga Antipova, Joseph Orgel.

02:15-02:40pm **13.11.03**
A One-dimensional Electron Density Map of Type I Collagen from Mouse Tail Tendon using X-ray Diffraction and Isomorphic Replacement Techniques. Simon Goodson, Justyn Regini, Keith Meek, Joseph Orgel.

02:40-03:00pm **13.11.04**
What Fiber Diffraction Can Tell Us About Cardiac Muscle Regulation. Tom Irving, HsiaoMan Hsu, Younss Ait Mou, Edward Allen, Kelly Schoenfelt, Pieter de Tombe.

03:00-03:30pm Coffee Break.

03:30-03:55pm **13.11.05**
Naturally Ordered Structural Materials. Jeffrey Deschamps.

03:55-04:10pm **13.11.06**
Non-enzymatic Glycation of Type I Collagen and its Effect on its Digestion by MMP-I. Rama Sashank Madhurapantula, Joseph Orgel, Olga Antipova.

04:10-04:30pm **13.11.07**
Targeting The Cd44-Hyaluronan Interaction Using Fragment-Based Drug Design. Li-Kai Liu, Barry Finzel.

04:30-05:00pm **13.11.08**
Novel Molecular Views of Nerve Myelin Using Microbeam X-ray Diffraction (XRD) and Neutron Diffraction (ND). Dan Kirschner, M. Burghammer, V. Cristiglio, B. Demé, A. Denninger, G. Le Duc, M. Palmisano, C. Riekel, M. Salmona.

Registration Desk	07:30am	Galleria Foyer	
Speaker Ready Room	07:30am	Griffin	
Council Meeting Room	07:30am	Carlton	
Exhibit Show	10:00am	Galleria Hall	
ACA Annual Business Meeting	5:00pm	Harbor II	
Poster Session T	5:30-7:30pm	Galleria Hall	

AW.03 Margaret C. Etter Early Career Award Presentation and Lecture - Emmanuel Skordalakes

George Phillips, Presiding
Harbor I

08:00-09:00am **AW.03.01**
Telomerase Structure Function. Emmanuel Skordalakes, Anthony Schuller, Andrew Gillis, Meghan Mitchell.

12.01 Etter Early Career Award Symposium

Eric Montemayor, Yulia Sevryugina, Presiding
Harbor I

09:00-09:15am **12.01.01**
A New Series of Compounds Formed from Substituted Pyridones and Pyridines with Dicarboxylic Acids. Kayla Sawyer, Bhupinder Sandhu, Marina S. Fonari, Tatiana V. Timofeeva.

09:15-09:30am **12.01.02**
Structural Analysis and Disorder Modeling of a New Terpenoid-Like Bischalcone. Hamilton Napolitano, William Fernandes, Lorraine Malaspina, Felipe Martins, Luciano Liäo, Ademir Camargo, Carlito Lariucci, Caridad Noda-Perezc.

09:30-09:45am **12.01.03**
The Potential of Lambda-Shaped Basic-Building Units Within Syntheses of Inorganic Noncentrosymmetric Crystals. Martin D. Donakowski, Romain Gautier, Kenneth R. Poeppelmeier.

09:45-10:00am **12.01.04**
Polymorphic Transitions for Highly-Oriented Crystals by Stereochemical Auxiliaries within Nanoscale Confinement. Qi Jiang, Chunhua Hu, Michael Ward.

10:00-10:30am Coffee Break

10:30-10:48am **12.01.05**
Crystal Structures of a Single Domain in PKGI Reveal the Molecular Mechanism of cGMP Selectivity. Gilbert Huang, Jeong Joo Kim, Albert Reger, Darren Casteel, Daniela Bertinetti, Robin Lorenz, Chi Zhao, Eui-Whan Moon, Friedrich Herberg, Choel Kim.

10:48-11:06am **12.01.06**
How Gaq Regulates PIP2 Hydrolysis: Molecular Mechanisms and Prospects for Drug Development. Angeline Lyon, Cassandra Boguth, Somnath Dutta, Vishan Dhamsania, Georgios Skiniotis, John Tesmer.

11:06-11:24am **12.01.07**
Structure-Based Design of Checkpoint Kinase 2 Inhibitors for Cancer Therapy. George Lountos, Andrew Jobson, Joseph Tropea, Christopher Self, Yves Pommier, Robert Shoemaker, David Waugh.

11:24-11:42am **12.01.08**
Structural Basis of Immune Evasion by HIV-1 Nef. Xiaofei Jia, Rajendra Singh, Stefanie Homann, Haitao Yang, John Guatelli, Yong Xiong.

11:42-12:00pm **12.01.09**
A Structural Comparison of Phylogenetically Distinct PreQ1 Riboswitches Provides Insight into Diverse Modes of Ligand Recognition and Gene Regulation. Joseph Liberman, Mohammad Salim, Joseph Wedekind.

09.04 Precipitates and Voids in Advanced Materials

Kenneth Littrell, Presiding
Burroughs

09:00-09:30am **09.04.01**
Study on the Early Stage of Precipitation in Steels by Combined use of SANS and SAXS. Masato Ohnuma, Yojiro Oba, Pawel Kozikowski, Suresh Koppoju.

09:30-10:00am **09.04.02**
Precipitation of Fine Alpha Precipitates in a Beta Titanium Alloy. James Coakley, Nicholas Jones, Kenneth Littrell, Vasilli Vorontsov, David Dye.

10:00-10:30am Coffee Break

10:30-11:00am **09.04.03**
Effect of Crystal Orientation on Mechanical Properties of Aluminum Alloys Produced by Various Casting Processes. Mitsuhiro Okayasu, Shuhei Takeuchi, Tetsuro Shiraishi.

11:00-11:15am **09.04.04**
Nanocrystallization in Bulk Metallic Glasses under Deformation. Alexandru Stoica, Dong Ma, Ken Litrell, Xun-Li Wang.

11:15-11:30am **09.04.05**
Multiscale Characterization of Pore Evolution in a Combustion Metamorphic Complex: Combining (Ultra) Small-Angle Neutron Scattering And Image Analysis. Hsiu-Wen Wang, Lawrence Anovitz, Lawrence Allard, Andrew Jackson, Gernot Rother, David Cole.

11:30-11:45am **09.04.06**
Small Angle Neutron Scattering Study of Porosity in Hexanitrostilbene. Ryan Wixom, Kenneth Littrell, James Browning.

11:45-12:00pm **09.04.07**
Measuring Thermal Stability of Nano-Precipitates in Advanced High-Strength Steel using SANS. Kenneth Littrell, Wan Chuck Woo, Zhili Feng, Lawrence Anovitz.

09.05 Complementary Techniques in Structural Biology

Arwen Pearson, Eddie Snell, Presiding
Burroughs

01:30-02:00pm **09.05.01**
All-Atom Molecular Dynamics Simulations of Peptide and Protein Crystals. David Case, Pawel Janowski, David Cerutti.

02:00-02:20pm **09.05.02**
Systems Biology in Prokaryote - Eukaryote Symbiosis: Single-Crystal Spectroscopy Correlated with X-ray Crystallography and Other Complementary Methods. Allen Orville, Feifei Li, Marc Allaire, Christian Roessler, Alexei Soares.

02:20-02:40pm **09.05.03**
The Role of pH in Triggering Structural Changes Towards Proper Infectivity in Adeno-associated Viruses. Joseph Yarbrough, Balasubramanian Venkatakrishnan, Robert McKenna, Mavis Agbandje-McKenna.

02:40-03:00pm **09.05.04**
Structural Interconversions Modulate Activity of *Escherichia coli* Ribonucleotide Reductase. Nozomi Ando, Edward Brignole, Christina Zimanyi, Michael Funk, Kenichi Yokoyama, Francisco Asturias, JoAnne Stubbe, Catherine Drennan.

03:00-03:30pm Coffee Break

03:30-04:00pm **09.05.05**
Layers of Reactivity. Dagmar Ringe.

04:00-04:20pm **09.05.06**
Solution NMR of a 463-Residue Phosphohexomutase: Domain 4 Mobility, Substates, and Ligand Binding Effects. Lesa Beamer, Akella Sarma, Asokan Anbanandam, Ritcha Mehra-Chaudhary, Allek Kelm, Yirui Wei, Yingying Lee, Mark Berjanski, Jacob Mick, Steven Van Doren.

04:20-04:40pm **09.05.07**
Structural Assembly of Bacterial Micro-reactors. Allan Pang, Martin Warren, Richard Pickersgill.

04:40-05:00pm **09.05.08**
Interaction and Crystallization Studies of the Periplasmic Proteins TraW and TrbC from the F plasmid Type IV Secretion System. Agnesa Shala, Gerald F. Audette.

10.01 Important Science From Small Molecule Structures

Alberto Albinati, Presiding
Harbor II

09:00-09:20am **10.01.01**
Hydrogen Interactions with Lewis Acid - Lewis Base Molecules: Storage and Catalysis. Mark Bowden, Abhi Karkamkar, Herman Cho, Greg Schenter, Kshitij Parab, Donald Camaioni, Doinita Neiner, Shawn Kathmann, Bojana Ginovska-Pangovska, Tom Autrey.

09:20-09:40am **10.01.02**
Dynamic Aspects of Crystal Structures from Temperature-dependent Neutron Diffraction Data. Silvia Chiara Capelli.

09:40-10:00am **10.01.03**
Dynamic Photocrystallography Across the Time Scales. Paul Raithby.

10:00-10:30am Coffee Break

10:30-10:50am **10.01.04**
Temperature and Pressure-Induced Phase Transitions in Metallocenes. Bruce Foxman, Logan Lorson, Shai Posner.

10:50-11:10am **10.01.05**
Why is the Ferroelectric Croconic Acid ($C_5H_2O_5$) so Dense ($p = 1.912$ g cm^{-3})? Alan Pinkerton, Vladimir Zhurov.

11:10-11:30am **10.01.06**
Structural Aspects of Transition Metal Reaction Mechanisms via Density Functional Theory. Michael Hall.

11:30-12:00pm **10.01.07**
Unexpected Structure Transformations and Resulting Reactivities upon Insertion of Au, Tl, or Pt into Nanosized CO/PR_3-Ligated Homopalladium Clusters. Lawrence Dahl, Evgueni Mednikov, Sergei Ivanov, Jeremiah Erickson.

10.02 Cool Structures

Jeanette Krause, Xiaoping Wang, Presiding
Harbor II

01:30-02:00pm **10.02.01**
Cool But Not Always Cold - The Interaction Between DNA and Ruthenium Complexes Reveal Interesting Structural Features. James Hall, Juan Sanchez-Weatherby, Kyra O'Sullivan, Hakan Niyazi, Graeme Winter, Thomas Sorensen, David Cardin, John Kelly, Christine Cardin.

02:00-02:30pm **10.02.02**
Transformation of the Structures and Properties of a Family of Metal Citrate Cubane Polymers. Elena Forcen-Vazquez, Larry R. Falvello, Isabel Mayoral, Fernando Palacio, Milagros Tomas.

02:30-03:00pm **10.02.03**
Cyanostars - Novel, Whole-Molecule-Disorder-Prone C5-Macrocycles with Powerful Anion Binding. Chun-Hsing Chen, Semin Lee, Amar Flood.

03:00-03:30pm Coffee Break

03:30-03:50pm **10.02.04**
Structural Manipulation Through Subtle Changes in Reaction Conditions for Zinc Alkylbisphosphonates. Kevin Gagnon, Zachary Beal, Alyssa Embry, Simon Teat, Abraham Clearfield.

03:50-04:10pm **10.02.05**
Structural Analysis of a Coumarin Ester: Mesomeric phenomenon or a case of Tautomerism? Lorraine Malaspina, Carlito Lariucci, William Fernandes.

04:10-04:20pm **10.02.06**
Study of Metal-Organic Frameworks Constructed from Different Secondary Building Units and Same Organic Ligands. Ying-Pin Chen, Andrey Yakovenko, Jinhee Park, Dawei Feng, Hong-Cai Zhou.

04:20-04:50pm **10.02.07**
Alteration of Molecular Structure of Metal-

Metal Bonded Dimers by Exposure to C_{60} Fullerene. Faye Bowles, Marilyn Olmstead, Alan Balch.

13.12 Complementary Methods

Michel Fodje, Presiding
Harbor III

09:00-09:30am **13.12.01**
Malignant Hyperthermia and Cardiac Arrhythmias: Crystal Structures and Pseudo-Atomic Models of the Ryanodine Receptor. Filip Van Petegem, Paolo Lobo, Lynn Kimlicka, Michael Yuchi, Kelvin Lau, Ching-Chieh Tung.

09:30-09:45am **13.12.02**
EMDataBank: Unified Data Resource for 3D Electron Microscopy. Catherine Lawson, Ardan Patwardhan, Matthew L. Baker, Brian Hudson, Ingvar Lagerstedt, Steven J. Ludtke, Grigore D. Pintilie, Gaurav Sahni, Raul Sala, Eduardo Sanz-Garcia, John D. Westbrook, Gerard J. Kleywegt, Helen M. Berman, Wah Chiu.

09:45-10:00am **13.12.03**
X-ray Crystallographic Structural Studies of the Metallochaperone-Like N-Terminal Domain (NmerA) of the Mercuric Ion Reductase MerA. Stephen Tomanicek, Alexander Johs, Mankaran Sawhney, Katherine Rush, Rachel Nauss, Susan Miller, Liyuan Liang.

10:00-10:30am Coffee Break

10:30-11:00am **13.12.04**
Structure and Dynamics of Arf GTPases and their GEFs. Jacqueline Cherfils.

11:00-11:25am **13.12.05**
Integrated Platform for Combined XRD and SONICC/TPE-UVF Measurements for Identification and Centering of Protein Crystals. Christopher Dettmar, Scott Toth, Michael Becker, Robert Fischetti, Garth Simpson.

11:25-11:45am **13.12.06**
X-ray Absorption Spectroscopy at the Canadian Light Source Beamline 08B1-1. Julien Cotelesage, Pawel Grochulski, Ingrid Pickering, Graham George, Michel Fodje.

11:45-12:00pm **13.12.07**
Structure Guided Design of the Smallest Infrared Fluorescent Phytochrome. Shyamosree Bhattacharya, Michele Auldridge, Katrina Forest.

13.13 Local Structure/Partially Ordered Systems

Katharine Page, Thomas Proffen, Presiding
Lewis

09:00-09:30am **13.13.01**
Local Atomic Structure Deviations from Average Structure of $Na_{0.5}Bi_{0.5}TiO_3$ Ferroelectric Ceramics. Elena Aksel, Jennifer S. Forrester, Katharine Page, Daniel P. Shoemaker, Jacob L. Jones.

09:30-09:45am **13.13.02**
Local Structure Models of Diffuse Scattering in Relaxor Ferroelectrics. Branton J. Campbell, Benjamin A. Frandsen, Va-Yee Vue, Matthew J. Gardner, Kevin D. Seppi.

09:45-10:00am **13.13.03**
Determining the Local Structural Changes Occurring During Geopolymerization Synthesis: A Combined Neutron and X-ray Pair Distribution Function Analysis. Breaunnah Bloomer, Claire White, Katharine Page.

10:00-10:30am Coffee Break

10:30-11:00am **13.13.04**
Simultaneous Fits to Local and Long-range Structure using Reverse Monte Carlo Simulations. Daniel Shoemaker, Duck Young Chung, Mercouri Kanatzidis.

11:00-11:30am **13.13.05**
Understanding Properties of Nanomaterials with Pair-Distribution Function Analysis. Mikhail Feygenson.

11:30-11:45am **13.13.06**
Quantitative NanoStructure Characterization

Using Atomic Pair Distribution Functions Obtained from Laboratory Electron Microscopes. A.M.M. Abeykoo, C.D. Malliakas, P. Juhas, E.S. Bozin, M. G. Kanatzidis, S.J.L. Billinge.

11:45-12:00pm **13.13.07**
Instrument Resolution Effects on the Pair Distribution Function of Nanomaterials. Claire Saunders, Thomas Proffen.

13.14 Extended Wavelength X-ray Crystallography

Robert Fischetti, Bi-Cheng Wang, Presiding
Harbor II

01:30-01:50pm **13.14.01**
Forward-looking Science Enabled by Optimized Extended Wavelength X-ray Sources for Macromolecular Crystallography: A General Introduction. Bi-Cheng Wang, John P. Rose, Gerold Rosenbaum, John Chrzas.

01:50-02:10pm **13.14.02**
The Upgrade Programme of Structural Biology at the European Synchrotron Radiation Facility. Christoph Mueller-Dieckmann, Sean McSweeney, Gordon Leonard, Alexandre Popov, Max Nanao, Matthew Bowler, Didier Nurizzo, Andrew McCarthy, Florent Cipriani, Pascal Theveneau.

02:10-02:30pm **13.14.03**
SAD Experiment using 2.7 Å Wavelength Performed at the Photon Factory. Naohiro Matsugaki, Yusuke Yamada, Leonard Chavas, Masahiko Hiraki, Noriyuki Igarashi, Seiji Okazaki, Hironori Suzuki, Masato Kawasaki, Ryuichi Kato, Soichi Wakatsuki.

02:30-02:45pm **13.14.04**
Got Halide? SAD Phasing in the Home Lab. J.W. Pflugrath, Vijaya Madakasira.

02:45-03:00pm **13.14.05**
Solving Protein Structures using Cu Kα Radiation from In-house X-ray Systems: Experiences with SAD Phasing. Matthew Benning.

03:00-03:30pm Coffee Break

03:30-03:50pm **13.14.06**
On the use of Longer X-ray wavelengths in Macromolecular Crystallography. Manfred Weiss.

03:50-04:10pm **13.14.07**
The Long-wavelength Macromolecular Crystallography Beamline at Diamond Light Source. Armin Wagner.

04:10-04:25pm **13.14.08**
Long-Wavelength Phasing at the Swiss Light Source. Meitian Wang, Sandro Waltersperger, Vincent Olieric, Guanya Peng, Clemens Schulze-Briese.

04:25-04:40pm **13.14.09**
New Tools for S-SAD Phasing. Zhi-Jie Liu, Wei Ding.

04:40-05:00pm **13.14.10**
Multi-crystal Native SAD Structural Analyses from Lower-energy Anomalous Diffraction. WayneA. Hendrickson, Qun Liu.

13.15 *In operando*/*in situ*/Parametric Studies

Antonio M. dos Santos, Presiding
Lewis

01:30-02:00pm **13.15.01**
Time-Resolved, *in situ* Studies of Chemical Syntheses using High Energy X- Ray Powder Diffraction. Dermot O'Hare, Saul Moorhouse.

02:00-02:20pm **13.15.02**
MOFs with Tunable Physical Properties: Insights in their Structure-property Relationships by *in-situ* X-ray Powder Diffraction Experiments. Mario Wriedt, Andrey A. Yakovenko, Julian P. Sculley, Hong-Cai Joe Zhou.

02:20-02:50pm **13.15.03**
Pulsed Magnetic Field Diffraction at the SNS. Garrett Granroth, S. Yoshii, H. Nojiri, K.A. Ross, B.D. Gaulin, J.P. Carlo, L. Santodonato, C.M. Hoffmann, A.A. Parizzi.

02:50-03:30pm Coffee Break

03:30-04:00pm **13.15.04**
In-situ Studies of Phase Transitions Driven by Oxygen Activity. Scott Misture.

04:00-04:20pm **13.15.05**
Crystallographic Insights into the High Capacity Oxoanion Cathode Material $LiFeBO_3$. Peter Khalifah, Shouhang Bo, Yuri Janssen, Derek Middlemiss, Clare Grey.

04:20-04:40pm **13.15.06**
In situ Studies Investigating Nanoparticle Ripening in Next-Generation Battery Materials. Kamila Wiaderek, Olaf Borkiewicz, Badri Shyam, Peter Chupas, Karena Chapman.

04:40-05:00pm **13.15.07**
Protein Dynamics Studied by Quasi-elastic Neutron Scattering. Xiang-qiang Chu, Eugene Mamontov, Coates Leighton, Manavalan Gajapathy, Joseph Ng, Kevin Weiss.

13.16 From Constructs to Crystals

George Lountos, Eric Ortlund, Presiding
Harbor III

01:30-02:00pm **13.16.01**
Maltose-Binding Protein and Tobacco Etch Virus Protease: Two Valuable Tools for the Production of Recombinant Proteins in *Escherichia coli*. David Waugh.

02:00-02:30pm **13.16.02**
Crystallization and Structure Determination of Membrane Proteins. Nicholas Noinaj, Susan Buchanan.

02:30-03:00pm **13.16.03**
Practical Concerns in the Production Through Structure Determination of Protein/Nucleic Acid Co-Crystals. Todd Green, Ming Luo.

03:00-03:30pm Coffee Break

03:30-03:45pm **13.16.04**
Microseed it! A Theoretical and Practical Exploration of Seed Stability and Seeding Techniques for Successful Protein Crystallization. Patrick Shaw Stewart, Stefan Kolek, Richard Briggs, Naomi Chayen, Peter Baldock.

03:45-04:00pm **13.16.05**
Improve The Efficiency and Reproducibility of the Protein Crystallization. Miki Senda, Toshiya Senda.

04:30-05:00pm **13.16.06**
Are Crystals Stochastic Moieties? Zygmunt Derewenda.

08.01 Would you Publish This?

Carla Slebodnick, Presiding
Burroughs **07:00-09:00pm**

Funding for this session provided, in part, by Crystallographic Resources, Inc.

08.01.01
Making the Decision to Publish. Phillip Fanwick.

08.01.02
Overcoming Difficulties Towards Publication. James Fettinger.

08.01.03
Riding a Lanthanide Raft in a Sea of Electron Density: Choppy Waters Make for a Rough Refinement. Louise N. Dawe, Muhammad U. Anwar, Laurence K. Thompson.

08.01.04
Crystal Structures of bis(3-X-N-Phthaloylalaninato)bis(N- Methylimidazole) Copper(II) Complexes. Approaches to Metal Based Quasiracemates. Mark A. Whitener, Hiral Patel, Mohit Singhal, Kraig A. Wheeler.

08.01.05
I am glad I Didn't Publish this; Refinement of Syn- and Anti- Isomers Against the Same Dataset. Kristin Kirschbaum, Stacy Gates, Alan Pinkerton.

08.01.06
For a Few Uglies More. Christine M. Beavers, Simon J. Teat.

Registration Desk	07:30am	Galleria Foyer
Speaker Ready Room	07:30am	Griffin
Council Meeting Room	07:30am	Carlton
Awards Banquet (ticket required) Reception 6:30pm	Dinner 7:30pm	Harbor II & III

AW.04 Supper Award Presentation and Lecture - Ron Hamlin

George Phillips, Presiding
Harbor I

08:00-09:00am **AW.04.01**
2-D X-ray Detectors - What do we Really Want and How can we Build It? Ron Hamlin.

TR.01-II Transactions: Transformations and Structural Oddities in Molecular Crystals: In Honor of Bruce M. Foxman

G. Diaz de Delgado, M. Hickey, K. Wheeler, Presiding
Harbor I

09:00-09:20am **TR.01-II.01**
Solid-state Chemistry in Pharmaceuticals. Magali Hickey.

09:20-09:40am **TR.01-II.02**
New Strategies for Exploring Crystallization Processes of Organic Materials. Kenneth Harris.

09:40-10:00am **TR.01-II.03**
Space Group Assignment and Evaluation of End-for-End Guest Disorder in $Cl(CH_2)_6CN$/Urea. Matthew Peterson, Kevin Pate, Brian Dinkelmeyer, Keith Alquist III, Mark Hollingsworth.

10:00-10:30am Coffee Break

10:30-10:50am **TR.01-II.04**
Turning on the Lights: A Perspective on the Value and Impact of Structural Information in Pharmaceutical R&D. Orn Almarsson.

10:50-11:10am **TR.01-II.05**
The Same But Different: Uric Acid Crystals Grown From Different Environments. Jennifer Swift, Janeth Presores, Amanuel Zellelow.

11:10-11:30am **TR.01-II.06**
Carboxylic Acids and Metal Carboxylates: Interesting Examples of Transformations and Structural Oddities. Graciela Diaz de Delgado,

11:30-11:50am **TR.01-II.07**
Channel Inclusion Compounds in Three, Four, and Five Dimensions. Mark Hollingsworth, Shane Nichols, Bo Wang, Keith Alquist, Angela Adams, Bertrand Toudic, Philippe Rabiller, Mickael Huard, Celine Mariette, Laurent Guerin.

03.02 General Interest II

Jeanette Krause, Presiding
Burroughs

01:30-01:50pm **03.02.01**
Mortar and Pestle - New Insights into Structural Changes in Crystals upon Milling from Combined SONICC Imaging and X-ray Diffraction. Garth Simpson, Debbie Wanapun, Umesh Kestur, Lynne Taylor.

01:50-02:10pm **03.02.02**
Enantioselective Crystallization of Racemic Pharmaceuticals on Chiral Molecular Films. Pranoti Navare, John Macdonald.

02:10-02:30pm **03.02.03**
Crystal to Crystal Transformation of Glycine. Chunhua Hu, Qi Jiang, Alexander Shtukenberg, Bart Kahr, Michael Ward.

02:30-02:50pm **03.02.04**
Exploiting the Tunable Wavelength Capabilities of Synchrotron Radiation for Small Molecule Single Crystal X-ray Crystallography. Karim Sutton, Richard Cooper, Kirsten Christensen, Amber Thompson, David Allan, Sarah Barnett.

02:50-03:30pm Coffee Break

03:30-03:50pm **03.02.05**
Moonlighting Proteins. Constance Jeffery.

03:50-04:10pm **03.02.06**
The First Structure of Immunodominant Vaccinia Envelop Protein D8 in Complex With La5-Mab Provides a Rare Insight into the B Cell Immune Response. Michael Matho, Matt Maybeno, Mohammed Rafii-El-Idrissi, Danielle Becker, Yan Xiang, Shane Crotty, Bjoern Peters, Dirk M. Zajonc.

04:10-04:30pm **03.02.07**
The SAS-6 Coiled Coil Structure and its Specific Interaction with SAS-5 Suggest A Mutual Regulation of the Two Proteins tn aentriole Assembly. Renping Qiao, Gang Dong.

04:30-04:50pm **03.02.08**
Analysis of Ribosomal Protein S13: Sequence Alignment Analysis Suggests Rooted Phylogenetic Tree. Alexander Merriman, William Duax.

11.01 Advanced Hardware and Applications

John Chrzas, John Rose, Presiding
Burroughs

09:00-09:15am **11.01.01**
Qmx, Asynchronous Data Collection for Macromolecular Crystallography. Howard Robinson, John Skinner.

09:15-09:30am **11.01.02**
PRIGo: A Novel Multi-Axis Goniometer for Macromolecular Crystallography at the Swiss Light Source. Sandro Waltersperger, Vincent Olieric, Marco Salathe, Claude Pradervand, Ezequiel Panepucci, Wayne Glettig, Clemens Schulze-Briese, Meitian Wang.

09:30-09:45am **11.01.03**
BAM-2 Automounter at CHESS. David Schuller, Mike Cook, Bill Miller, Scott Smith, D.M.E. Szebenyi.

09:45-10:05am **11.01.04**
Advances in Automation for Macromolecular Crystallography Experiments at SSRL. Aina Cohen.

10:05-10:30am Coffee Break

10:30-10:45am **11.01.05**
Pixel Detectors: New Developments. Christian Bronnimann.

10:45-11:05am **11.01.06**
Integration of the Dectris Pilatus 6MF PAD detector at NE-CAT. Malcolm Capel, Kanagalaghatta Rajashankar, Frank Murphy, Sreve Ealick.

11:05-11:25am **11.01.07**
Next Generation Large Integrating X-ray Detectors-Frame-Transfer CCDs. Michael Blum.

11:25-11:40am **11.01.08**
Fast Detector Implementation Plans at SER-CAT. John Chrzas, James Fait, Zheng-Qing (Albert) Fu, John Gonczy, Zhongmin Jin, John Rose, Bi-Cheng Wang.

11:40-12:00pm **11.01.09**
The New Dual Mode Pixel Array Detector. Ron Hamlin, Tom Hontz, Chris Nielsen.

13.18 Public Domain Software

Xiaoping Wang, Presiding
Harbor II

09:00-09:20am **13.18.01**
An Update on Current and New Crystal Structure Analysis Tools in PLATON. Anthony Spek.

09:20-09:40am **13.18.02**
The Development of GSAS-II. Robert Von Dreele.

09:40-10:00am **13.18.03**
Olex2[1] and smtbx[2]: One Package. Oleg Dolomanov, Luc Bourhis, Richard Gildea, Judith Howard, Horst Puschmann.

10:00-10:30am Coffee Break

10:30-11:00am 13.18.04
SHELXL - 2012. GeorgeM. Sheldrick.

11:00-11:20am 13.18.05
CRYSTALS: Teaching an Old Dog New Tricks. Richard Cooper.

11:20-11:40am 13.18.06
AMPLE - A Software Tool For The Employment of *ab initio* Protein Structure Modelling Techniques in Molecular Replacement. Ronan Keegan, Ronan Keegan, Jaclyn Bibby, Daniel Rigden, Martyn Winn, Olga Mayans.

11:40-12:00pm 13.18.07
New Python-Based Software for Data Reduction. Nicholas Sauter, David Waterman, Graeme Winter.

13.19 Functional and Emerging Materials and Technology

Craig Bridges, James Kaduk, Presiding
Lewis

09:00-09:30am 13.19.01
Exploratory Crystal Growth: Oxides from Hydroxides, Hydroxometallates from Hydrofluxes, and Strategies for Controlling Metal Oxidation States. Hans-Conrad zur Loye, W. Michael Chance, Qingbiao Zhao, Daniel Bugaris, Jeongho Yeon.

09:30-10:00am 13.19.02
Charting the Fluctuating Ir^{4+}-dimer Map Across the Phase Diagram of $Cu(Ir_{1-x}Crx)_2S_4$ ($0<x<0.6$). Emil Bozin.

10:00-10:30am Coffee Break

10:30-10:50am 13.19.03
The High Pressure Behaviour of the 3D Copper Carbonate Framework $\{[Cu(CO_3)_2](CH_6N_3)_2\}_n$. Elinor Spencer, Nancy Ross, Ross Angel.

11:10-11:30am 13.19.05
Structural Transformations that Effects Porosity in Metal Phosphonates. Tiffany Kinnibrugh, Ayi Anyama, Vladimir I. Bakhmutov, Abraham Clearfield.

11:30-11:50am 13.19.06
Structure Study of Molybdate Glasses by Neutron and X-ray Diffraction and RMC Modeling. Margit Fabian, Erzsebet Svab, Anna Llobet, Martin von Zimmermann.

11:50-11:10am 13.19.04
Study of Metal-Organic Frameworks by X-ray Powder Diffraction: Analysis of Structure Envelope Difference Density. Andrey Yakovenko, Mario Wriedt, Zhangwen Wei, Jinhee Park, Hong-Cai Zhou.

11:50-11:55am 13.19.08
Optical Characterization of Newly Synthesized Chiral Compounds. Max Kaganyuk, Werner Kaminsky, Meghana Rawal.

13.20 Membrane Proteins from Start to Finish

Vadim Cherezov, Presiding
Harbor III

09:00-09:30am 13.20.01
The Structure of Components of a Multi-component Integral Membrane Pump of the HME RND Family. Robert Stroud, John Pak, Chantal Eckende, John Lee, Joseph D. O'Connell III, Fabien DeAngelis, Cedric Bauvois, Cedric Govaerts, Jean-Marie Ruysschaert, Guy Vandenbussche.

09:30-10:00am 13.20.02
15 Years Lipidic Cubic Phase Crystallization: a Critical Appraisal. Ehud Landau.

10:00-10:30am Coffee Break

10:30-10:55am 13.20.03
A Comparison of Crystallization Techniques for the Outer Membrane Proteins Intimin and Invasin. Susan Buchanan, James Fairman, Nicholas Noinaj, Travis Barnard, Wei Liu, Vadim Cherezov.

10:55-11:20am 13.20.04
Advanced Beamline Tools Aid Structure Determination from Micro-Sized Crystals of

Macromolecules and Complexes. Robert F. Fischetti, C.M. Ogata, R. Sanishvili, V. Nagarajan, M. Becker, S. Stepanov, M. Hilgart, S. Pothineni, S. Xu, O. Makarov, D. Yoder, J.L. Smith.

11:20-11:40am 13.20.05
Fusion Partner Toolchest for the Stabilization and Crystallization of G Protein-Coupled Receptors. Eugene Chun, Aaron Thompson, Wei Liu, Christopher Roth, Vsevolod Katritch, Vadim Cherezov, Laura Heitman, Adriaan IJzerman, Michael Hanson, Raymond Stevens.

11:40-12:00am 13.20.06
Structure Determination of a Na-Pumping Membrane Pyrophosphatase - Something Old, Something New. Tommi Kajander, Juho Kellosalo, Konstantin Kogan, Adrian Goldman.

13.21 Crystallographic Information in Pharmaceutical Research & Development

Magali Hickey, Matthew Peterson, Presiding
Harbor II

01:30-01:50pm 13.21.01
Getting Physical to Fix Pharma: Leveraging Calorimetric and Crystallographic Data to Understand and Improve the Performance of Pharmaceuticals. Patrick Connelly.

01:50-02:10pm 13.21.02
Isostructurality in Pharmaceutical Salts: How Often and How Similar? Peter Wood, Mark Oliveira, Andrina Zink, Magali Hickey.

02:10-02:30pm 13.21.03
Structural Insights from Variable Temperature Powder X-Ray Diffraction Data. Eugene Cheung, Mary Stanton, Matthew Peterson.

02:30-02:50pm 13.21.04
A First Principles Treatment of Polymorphism in Molecular Crystals Using Dispersion-Corrected Density Functionals. Noa Marom.

02:50-03:30pm Coffee Break

03:30-03:50pm 13.21.05
The Role of Small Molecule Crystallography in Pharmaceutical Product Designs. Dedong Wu.

03:50-04:10pm 13.21.05
Studies of the Single-Crystal X-ray Diffuse Scattering in Pharmaceuticals. Eric Chan, Darren Goossens, Aidan Heerdegen, T. Richard Welberry.

04:30-04:50pm 13.21.08
Conformationally Restricted Crystallization of an Opioid Modulator. Mark Oliveira, Mark Tawa, Renato Chiarella, Scott Duncan, Juan Alvarez, Magali Hickey, Julius Remenar, Örn Almarsson.

13.22 Structure-Guided Drug Discovery

Stephen K. Burley, Magali Hickey, Presiding
Harbor III

01:30-01:45pm Opening Remarks

01:45-02:15pm 13.22.01
Specific Targeting of Epigenetic Effector Domains of the Bromodomain Family. Stefan Knapp.

02:15-02:30pm 13.22.02
Crystal Structures of Human Farnesyl Pyrophosphate Synthase in Complex with a Novel Bisphosphonate Inhibitor with Anti-Cancer Activity. Jaeok Park, Yih-Shyan Lin, Youla S. Tsantrizos, Albert M. Berghuis.

02:30-03:00pm 13.22.03
Data Management of Small Molecule Ligands, Antibiotics, and Peptide Inhibitors in the PDB. Helen Berman, Shuchismita Dutta, Zukang Feng, Kim Henrick, Miri Hirshberg, Chenghua Shao, John Westbrook, Jasmine Young, Marina Zhuravleva.

03:00-03:30pm Coffee Break

03:30-03:45pm **13.22.04**
Structure Based Drug Design of Imidazo [1,2-a] Pyrazine inhibitors against Aurora Kinase. Alan Hruza, Andrea Basso, Patrick Curran, Sara Esposite, Kimberly Gray, Daniel Hicklin, Mengwei Hu, Jennifer Jones, Angela Kerekes, Lianzhu Liang.

03:45-04:00pm **13.22.05**
Covalent Inhibition of Macrophage Migration Inhibitory Factor. Gregg Crichlow, Elias Lolis.

04:15-04:45pm **13.22.07**
Towards Chemical Interventions against Amyloid Diseases. David Eisenberg, Meytal Landau, Stuart Sievers, Anni Zhao, Lin Jiang, Luki Goldschmidt, Arthur Laganowsky, Cong Liu, Magdalena Ivanova, Angela Soriaga, Howard Chang, Daniel Anderson, Michael Sawaya, Duilio Cascio.

04:45 - 05:00pm Closing Remarks

13.23 Data Collection with the Pros

Edward Collins, Andew Torelli Presiding
Harbor I

01:30-03:00pm **13.23.01**
Optimal Diffraction Experiment. Zbigniew Dauter.

03:00-03:30pm Coffee Break

03:30-04:00pm **13.23.02**
Signal vs Noise: and How to Tip the Balance in Your Favor. James Holton.

04:00-04:30pm **13.23.03**
Data Collection with 6 Million Detectors. Raj Rajashankar, Igor Kourinov, Malcolm Capel, Steve Ealick.

13.24 Phase Transitions in Inorganic Systems

Branton Cambell, Presiding
Lewis

01:30-02:05pm **13.24.01**
Rational *ab initio* Modeling for Polytypic Transformations and Phase Stability in Kaolin Minerals. Patrick Mercier, Yvon Le Page.

02:05-02:40pm **13.24.02**
Petalite $LiAlSi_4O_{10}$ Crystal Under High Pressure up to 5 GPa. Nancy Ross, Jing Zhao, Elinor Spencer, Bryan Chakoumakos.

02:40-03:00pm **13.24.03**
The Role of a La Dopant in Inhibiting the gamma-to-alpha Al_2O_3 Phase Transition. Stacey Smith, Baiyu Huang, Calvin Bartholomew, Juliana Boerio-Goates, Brian Woodfield, Branton Campbell.

03:00-03:30pm Coffee Break

03:30-04:10pm **13.24.04**
Magnetic and Crystallographic Structure Evolution in Manganates and Vanadates. Mario Bieringer.

04:10-04:35pm **13.24.05**
Structural Coherence and Ferroelectric Order in Submicron and Nano-Sized Multiferroic $YMnO_3$. Saurabh Tripathi, Valeri Petkov.

04:35-05:00pm **13.24.06**
"Thermochromic" Phase Transitions in $(1,2,6\text{-Trimethylpyridinium})_2CuX_4$ Salts (X = Cl, Br). Marcus Bond, Annette Kelley, Allison Talley.

SP.02 The History of Structural Biology

George Phillips, Presiding
Harbor II

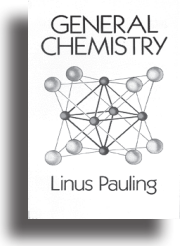
5:15pm Donald Caspar

THURSDAY AUG. 2

2013 Hawaii Meeting Planning Session

08:30am **Burroughs**

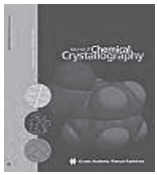
POSTER PRIZES



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.

Canadian National Committee for Crystallography (CNCC)



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 (www.rsc.org/Publishing/Journals/CE/about.asp) shortly after the conclusion of the ACA meeting.

RSC | Advancing the Chemical Sciences

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.

POSTER HANGING INSTRUCTIONS

Posters beginning with **S** should be assembled before 11:00am on Sunday and be removed at the conclusion of the poster session at 7:30pm.

Posters beginning with **M** should be assembled before 11:00am on Monday and be removed at the conclusion of the poster session at 7:30pm.

Posters beginning with **T** should be assembled before 11:00am 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

S-01
Structural Studies of SHP-1 Protein Tyrosine Phosphatase Substrate Recognition. Nilda Alicea-Velazquez, Titus Boggon.

S-02
The MCSG Suite: A Diverse and Productive Approach to Initial Sparse Matrix Crystallization Screening. Melanie A. Adams-Cioaba, Kateryna Podzelinska, Morten O.A. Sommer.

S-03
Accumulation of Silent but Enabling Amino Acid Substitutions Directed the Evolutionary Pathway by which the DNA Binding Specificities of the Steroid Hormone Receptors Diverged. Michael Murphy, Jamie Bridgeham, Joe Thornton, Eric Ortlund.

S-04
Structure-Driven Analysis into the General Mechanisms of Retroviral Entry. Halil Aydin, Jonathan D. Cook, Brianna Smrke, Jeffrey E. Lee.

S-05
Structural and Functional Studies of Hepatitis C Virus RNA dependent RNA Polymerase. Chandni Rao, Caitlin Kaczowka, Isabelle Barrette-Ng, Kenneth Ng.

S-07
The Crystal Structure of the Dimerization and Docking Domain of cGMP Dependent Protein Kinase Iα Reveals the Molecular Details for Redox-Sensing. Albert Reger, Robin Lorenz, Kimoon Ryu, Elaine Guo, Matthew Yang, Darren Casteel, Choel Kim.

S-08
Membrane Protein Production Strategies at the Transmembrane Protein Center. Craig Bingman, Shin-ichi Makino, David Aceti, Khaled Aly, James Bangs, Emily Beebe, Baron Chandra, Katrina Forest, John Primm, Brian Fox.

S-09
X-ray Crystal Structure of α-L-Fucosidase GH29 from *Fusarium graminearum* Reveals a Novel βγ Crystallin-like Domain as a Putative New Carbohydrate- Binding Module. Hongnan Cao, Jonathan Walton, Phil Brumm, George Phillips.

S-10
GridZilla: A Software Tool to Design and Create Crystallization Screening Grids by Hand or Using Liquid Handling Automation. Hari Jayaram.

S-11
Structural and Biochemical Characterization of Human Adenylosuccinate Lyase (ADSL) and ADSL Deficiency Associated Mutations. Michelle Deaton, Stephen Ray, Glenn Capodagli, Lauren Calkins, Lucas Sawle, Kingshuk Ghosh, David Patterson, Scott Pegan.

S-12
A Robotic Sample Changing System for Queued Diffraction Experiments With Decoupled Evaluation. Frank von Delft, Dan Herodes, Robert Lancaster, Florian Hauser,

Brian Michell, Stephen Leo, Nathan Wright, Tobias Krojer, Matt Benning, Roger Durst.

S-13
Temperature Dependence of Thermolysin Kinetic and Structural Phase Transitions. Ming Dong, Timothy Koblish, Brian Bahnson.

S-14
Sulfur Functional Groups for Cocrystallisation. Kevin Eccles, Kevin Eccles, Robin Morrison, Anita Maguire, Simon Lawrence.

S-15
Investigating the Role of the C-terminal Tail of PLP Synthase. Amber Smith, Janet Smith.

S-16
Monitoring the Oxidation States of Metals/Ions in Crystals. Palani Kandavelu, Hua Zhang, Zheng-Qing (Albert) Fu, Lirong Chen, John Chrzas, John P. Rose, Bi-Cheng Wang.

S-17
Crystal Structure of *Pseudomonas putida* Chlorocatechol 1,2-dioxygenase. Structural Basis for Substrate Uptake and Specificity. Joane Kathelen Rustiguel Bonalumi, Daniela Spuri Bernardi, Renata Fonseca Vianna Lopez, Maria Cristina Nonato.

S-18
Crystallography in Undergraduate Research: Correlating Thermal Motion Analysis using X-ray Diffraction, Raman Spectroscopy and Molecular Modeling. Wayne Pearson, Rhett Barker.

S-19
Using X-ray Crystallography to Design of Isoform Specific Carbonic Anhydrase Inhibitors. Mayank Aggarwal, Melissa Pinard, Claudiu Supuran, Robert McKenna.

S-20
Neutron and X-ray Structures of Crambin at Ultra-high Resolution Elucidate Water and Side Chain Dynamics and Relate to Function. Martha Teeter.

S-21
Conformationally Restrained North-methanocarba-2'-deoxyadenosine Corrects the Error-Prone Nature of Human DNA Polymerase Iota. Surajit Banerjee, Amit Ketkar, Maroof Zafar, Victor Marquez, Martin Egli, Robert Eoff.

S-22
New Approaches to Time-Resolved Structural Studies of Macromolecules. Briony Yorke, Arwen Pearson, Michael Webb, Emanuele Paci, Robin Owen.

S-23
Kinetic and Structural Characterization of Thermostabile Variants of Human Carbonic Anhydrase II. Christopher Boone, Zoe Fisher, Shyamasri- Biswas, Balasubramanian Venkatakrishnan, Mayank Aggarwal, Chingkuang Tu, Mavis Agbandje-McKenna, David Silverman, Robert McKenna.

S-24
Thermal Cleavage of Cyclobutane Rings in the Photodimerized Coordination Polymeric Sheets. Anjana Chanthapally, Jagadese J. Vittal.

S-25
Structure of Family 19 Chitinase Enzyme from Zea Mays at 2.0 Å Resolution. . Marcia Chaudet, Todd A. Nauman, Neil Price, David R. Rose.

S-26
Preparation and Characterization of Nano-Structures of Transition Metal Oxides. Rumana Jahan, Altaf Hussain.

S-27
Structural and Kinetic Studies of a Novel Alpha Carbonic Anhydrase expressed in *Thiomicrospira crunogena* gammaproteobacterium. Natalia A. Diaz-Torres, Shyasmasri Biswas, Chingkuang Tu, David N. Silverman, Kathleen M. Scott, Robert McKenna.

S-28
Effect of Ligand Structural Isomerism in For-

mation of Calcium Coordination Networks. Anna Plonka, Debasis Banerjee, John B. Parise.

S-29
Crystallographic Studies of Werner Syndrome DNA Helicase. Ken Kitano, Sun-Yong Kim, Toshio Hakoshima.

S-30
Investigation of the Composition and Structure of Ferrous and Manganese- Ferrous Minerals Out of Lake-Marsh Ores. Anton Chuev, Nikolai Fedorchuk, Maria Petrova.

S-31
Structural Insights into the Mechanism of Enzymatic Degradation of Toxoflavin. Michael Fenwick, Benjamin Philmus, Sameh Abdelwahed, Howard Williams, Tadhg Begley, Steven Ealick.

S-32
Crystal Structures of Group 1 Citrate Salts. James Kaduk, Alagappa Rammohan.

S-33
Structural Determinants of Substrate Specificity in a Nitrilase Superfamily Amidase. Serah Kimani, Trevor Sewell.

S-34
Service Crystallography and Remote Access at the Australian Synchrotron Macromolecular Crystallography Beamlines. Christine Gee, David Aragao, Santosh Panjikar, Nathan Cowieson, Alan Riboldi-Tunnicliffe, Rachel Williamson, Tom Caradoc-Davies.

S-35
The Structure of Quinone Reductase 2 Changes Upon Reduction of FAD and Binding of the Anti-malarial Drug Chloroquine. Kevin Leung, Brian Shilton.

S-36
A User Facility for Acoustic Specimen Preparation and Fast Library Screening. Alexei Soares, Christian Roessler, Marc Allaire, Allen Orville, Matthew Engel, Krystal Cole, Joseph Olechno, Richard Ellson, Richard Stearns, Sammy Datwani.

S-37
The Structure and Function of S*treptomyces bingchenggensis* Acetoacetate Decarboxylase. Lisa Mueller, Nicholas Silvaggi.

S-38
SAXS Studies on Human and Yeast Leukotriene A4 Hydrolase: Important for Revealing Comparison of a Bifunctional Catalytic Mechanism. Mahmudul Hasan, Agnes Rinaldo-Matthis, Jesper Haeggstrom, Marjolein Thunnissen.

S-39
Crystal Structure of a Novel Branched-Chain Amino Acid Dioxygenase from *Burkholderia ambifaria* AMMD. Huimin Qin, Takuya Miyakawa, Akira Nakamura, Takashi Kawashima, Makoto Hibi, Jun Ogawa, Masaru Tanokura.

S-40
Advances in Hardware for Small Angle Scattering. Matthew Benning, Vernon Smith.

S-41
Five-domain α-Amylase from *Bacillus subtilis*. Mae Saldajeno, Rick Bott.

S-42
Recent Advances at the SIBYLS Beamline (ALS 12.3.1): Small Angle X-ray Scattering and Macromolecular Crystallography. Scott Classen, Greg Hura, Michal Hammel, Rob Rambo, Ivan Rodic, John Tainer.

S-43
Structure of *Clostridium botulinum* BcmE, a Thiamin-Degrading Enzyme, Co-Crystallized with Thiamin. Megan Sikowitz, Brateen Shome, Tadhg Begley, Steven Ealick.

S-44
A Nanoscopic View of a Microscopic Sodium Caseinate O/W Emulsion: Protein Micellar Structure and Emulsion Physical Behavior.

Christian Huck-Iriart, Maria Lidia Herrera, Roberto J. Candal, Cristiano L.P. Oliveira, Iris L. Torriani.

S-45
The Structural Basis of Protein Phosphatase 2 Å Methylation. Vitali Stanevich, Li Jiang, Kenneth Satyshur, Yongna Xing.

S-47
Structural Insights into a Novel Class of N-linked Protein Glycosylation by the *Actinobacillus pleuropneumoniae* HMW1C-Like Protein. Hye-Jeong Yeo, Fumihiro Kawai, Kyoung-Jae Choi, Sue Grass, Youngchang Kim, Joe St. Geme.

S-48
Probing Cooperative Translational Motions in Channel Inclusion Compounds of Urea. Keith Alquist, Kevin L. Pate, Mike L. Peterson, Roman B. Gajda, Brian D. Dinkelmeyer, Benjamin L. Champion, Mark D. Hollingsworth.

S-49
Crystal Structure of *Methanococcus jannaschii* Mj0601, a Putative Thiazole Synthase. Xuan Zhang, Bekir Eser, Tadhg Begley, Steven Ealick.

S-50
Crystal and Molecular Structure Analyses of the N-acylhydrazone Derivatives. Rosane Castro, Cinthia Correa, Jose Sabino, Lidia Lima, Daniel Amaral, Amanda Silva, Eliezer Barreiro.

S-51
Ligand Modifications to Reduce the Relative resistance of Multi-Drug Resistant HIV-1 Protease. Tamaria Dewdney, Yong Wang, Zhigang Liu, Samuel Reiter, Joseph Brunzelle, Iulia Kovari, Ladislau Kovari.

S-52
Optical Characterization of Newly Synthesized Chiral Compounds. Max Kaganyuk, Werner Kaminsky, Meghana Rawal.

S-53
Crystal Structure Analysis of Nectin and Nectin-Like-Molecule Family (II). Mamoru Suzuki, Hirotaka Narita, Atsushi Nakagawa.

S-55
Synthesis and Crystal Chemistry of Ti-Doped Mayenite. Sabina Ude, Claudia Rawn .

S-56
Cooperative Guest-Host-Guest Recognition in Ferroelastic and Ferroelectric Calixarenes. Bo Wang, Matthew Peterson, Shane Nichols, Eric Cha, Mark Hollingsworth.

S-57
Studies of Internal Strain in Cast Uranium with Refined Grain Size. Elena Garlea, R.L. Bridges, V.O. Garlea, M.A. Hemphill, J.S. Morrell.

S-58
Crystal Structure of a 16 nm, Half-megadalton Protein Cage Designed by Fusing Symmetric Oligomeric Domains. Yen-Ting Lai, Duilio Cascio, Todd Yeates.

S-59
Crystal Structure of ε-UO3. Claudia Rawn, Jared Johnson, Melanie Kirkham, Roberta Peascoe, Ashfia Huq.

S-60
Crystallography of a Lewis-Binding Norovirus, Elucidation of Strain-Specificity to the Polymorphic Human Histo-Blood Group Antigens. Xuemei Li, Yutao Chen, Ming Tan, Ming Xia, Ning Hao, Xuejun C Zhang, Pengwei Huang, Xi Jiang, Zihe Rao.

S-61
Structural Studies of Streptomycin Resistant and Dependent Ribosomes. Hasan Demirci, Steven Gregory, Frank Murphy, Gerwald Jogl, Albert Dahlberg.

S-62
High School Program - Acton-Boxborough Regional High School. Brian Dempsey, Ame-

lia Feinberg-Eddy, Aaron Mathieu, Nikita Kahn.

S-63
Structural Basis for the Design of New Immunosuppressants. Simina Grigoriu, Rachel Bond, Rebecca Page, Jenn Chen, Martha Cyert, Wolfgang Peti.

S-64
Engineered Legume Lectins with Altered Quaternary Structures. Dmitry Rodionov, Albert Berghuis.

S-65
Crystal Structure of a Type III Effector Protein in Complex with its Chaperone. Andrei Halavaty, Dominika Borek, Gregory H. Tyson, Ludmilla Shuvalova, George Minasov, Zbyszek Otwinowski, Alan R. Hauser, Wayne F. Anderson.

S-66
Fragment-Based Optimization of an Inhibitor of Mycobacterium Tuberculosis BioA. Ran Dai, Todd Geders, Barry Finzel.

S-67
The Crystal Structure of the Holoenzyme Shiga Toxin 2 with a Bound Disaccharide Inhibitor. Michael James, Jiang Yin, Jared Jacobson, Pavel Kitov, George Mulvey, Glen Armstrong, David Bundle.

S-68
Specificity, Structure, Dynamics and Inhibition of Tiam1 PDZ Domain/Syndecan1 Complex. Xu Liu, Tyson Shepherd, Ann Murray, Ernesto Fuentes.

S-69
Structure and Function of a Novel Phosphorylated Domain in the SF1 / U2AF65 Splicing Factor Complex. Wenhua Wang, Ankit Gupta, William Bauer, Valerie Manceau, Michael Green, Alexandre Maucuer, Clara Kielkopf.

S-71
Finding and Keeping Small Crystals in the Beam. Micheal Becker, Craig Ogata, Stephen Corcoran, Derek W. Yoder, Sergey Stepanov, Mark Hilgart, Oleg Makarov, Ruslan Sanishvili, Shenglan Xu, Dale Ferguson, Nagarajan Venugopalan, Christopher Dettmar, Scott Toth, Jeremy Madden, David J. Kissick, Garth J. Simpson, Janet L. Smith, Robert F. Fischetti.

S-72
SAXS as a Probe of Ice Nucleation and Growth in Bulk Solutions. Jesse Hopkins, Matthew Warkentin, Robert Thorne.

S-73
Mosquito© Crystal and Mosquito© LCP: Fast, Reliable Automation of Protein Crystallisation Drop Set-up . Ben Schenker, Joby Jenkins, David Smith, Wendy Gaisford.

S-74
Tools for High-Throughput Structural Biology at the Joint Center for Structural Genomics. Glen Spraggon, Heath Klock, Mark Knuth, Carol Farr, Scott Lesley.

S-75
Non-Bonded Contacts in Protein Crystal Structures: All-Atom Refinement at Moderate Resolution with PrimeX. Jeffrey Bell, Kenneth Ho, Ramy Farid.

S-76
A Convenient and General Expression Platform for the Production of Secreted Proteins from Human Cells. Jonathan Cook, Halil Aydin, Farshad C. Azimi, Jeffrey E. Lee.

S-77
Application of the Quantum Mechanics Crystallographic Refinement Protocol to Improve Ligand Structural Properties and Strain Energy. Oleg Borbulevych, Lance M. Westerhoff.

S-78
ISPyB - An Information Management System for Synchrotron MX Experiments. Karl Erik Levik, Solange Delageniere, Marjolaine Bodin, Martin A. Walsh, Elspeth J. Gordon, Alun W. Ashton.

S-79
Comparison of Electrostatic Properties of Four Macrolide Antibiotics. Birger Dittrich, Alke Meents.

S-80
Natural User Interface System for Crystallographic Visualization and Manipulation. Lagnajeet Pradhan, Hyun-Joo Nam.

S-81
Homochiral and Racemic Clusianone-Type Natural Products from Hypericum Species. Frank Fronczek, Omar Christian, Sara Crockett.

S-82
CCP4 6.3 - new software and improved software tools for protein crystallography.. Marcin Wojdyr, Charles Ballard, Eugene Krissinel, Ronan Keegan, David Waterman, Andrey Lebedev, Ville Uski.

S-83
Hydrogen Bonding and Conformation in Salts of Diclofenac. Carl Schwalbe, Miren Ramirez, Barbara Conway, Peter Timmins.

S-84
Chem-BLAST: Algorithms and Implementation of Chemical Semantic Web for Chemical Crystallography. Talapady Bhat.

S-86
Neutron Structure of the Clinical Drug Acetazolamide, Bound to Human Carbonic Anhydrase II. Zoe Fisher, Mayank Aggarwal, Chris Boone, David Silverman, Robert McKenna.

S-87
Investigation of the Phase Changes from a Twinned to Single Crystal by X-ray Diffraction and Differential Scanning Calorimetry. Gregory Rohde, Victor Young, Michael Carney.

S-88
Heightened Structural and Mechanistic Characterization of bsTrpRS. Tishan Williams, Li Li, Violetta Weinreb, Charles Carter.

S-89
Solid-state Diels-Alder Cycloaddition via Charge-Transfer Complexes: Reaction of N,N'-bis(propylimino)-1,4-dithiin with 2-acetyl-anthracene. Sanaz Khorasani, Manuel Fernandes.

Monday Posters

M-01
Sample Loop Vibration: Stress Testing Protein Sample Mounting Loops for Rigidity. Eandy Alkire, Frank Rotella, Norma Duke.

M-02
Using RMSD to Compare the 3D Structures of Active Sites for Protein Function Prediction. Madolyn MacDonald, Paul Craig, Herbert Bernstein.

M-03
Structural Features of the Dihydrolipoamide Dehydrogenase E3 Component from the *E. coli* Pyruvate Dehydrogenase Complex. K. Chandrasekhar, P. Arjunan, Y.H. Park, J. Song, F. Jordan, W. Furey.

M-04
Cofactor Specificity and Binding of IDH by Mutagenesis and X-ray Crystallography. Drew Bertwistle, Karin Straaten, Hari Aamudalapalli, David R.J. Palmer, David A.R. Sanders.

M-05
Crystal Structure Analysis of Solute Binding Proteins for Transport of Aromatic Products. Changsoo Chang, Jamey Mack, Sarah Zerbs, Frank Collart, Andrzej Joachimiak.

M-06
Structure Activity Characterization of the Sulfide: Quionone Oxidoreductase Variants. Maia Cherney, Yanfei Zhang, Michael James, Joel Weiner.

M-07
Structure-Based Evolution of β-Glucuronidase

for Antibody-Directed Enzyme Prodrug Therapy. Sean Dalrymple, Rajendra Jagdhane, David Palmer, David Sanders.

M-08
Crystal Structures and Small-angle X-ray Scattering Analysis of UDP-galactopyranose mutase from the Pathogenic Fungus *Aspergillus fumigatus*. Richa Dhatwalia, Harkewal Singh, John Tanner.

M-09
Crystal Structure of Rv2717c at 1.5Å Resolution. Li-Wei Hung, Chang-Yub Kim, Brent Segelke, Minmin Yu, Emily Z. Alipio, Thomas C. Terwilliger.

M-10
Crystal Structure of the Carboxyl Cyclic Nucleotide Binding Domain of *P. falciparum* cGMP Dependent Protein Kinase. Jeong Joo Kim, Choel Kim, Eduardo Sanabria Figueroa, Albert S. Reger.

M-11
Structural Studies of three Oxidoreductases. Seetharaman Jayaraman, A.P Kuzin, F. Forouhar, S.M Vorobiev, M. Su, H. Neely, M. Abashidze, Y. Chen, S. Lew, R. Xiao.

M-12
Structural and Kinetic Investigations of the Dynamic Plasticity in the Active Site of the Carboxyl Transferase Domain in Pyruvate Carboxylase. Adam Lietzan, Martin St. Maurice.

M-13
Structural Analysis of Two Contact-Dependent Growth Inhibiting Complexes. Robert Morse, Elias Gerrick, Angelina Iniguez, Kiel Nikolakakis, Christopher Hayes, Celia Goulding.

M-14
Structural Rearrangements Associated with Bond Formation in Schiff-Base Forming Enzymes. Samuel Light, Mark-Eugene Duban, George Minasov, Wayne Anderson.

M-15
The Crystal Structure of the Circadian Clock Protein KaiA with Bound 2,5-Dibromo-3-Methyl- 6-Isopropyl-p-Benzoquinone (DBMIB), a Redox-Active Cofactor. Rekha Pattanayek, .

M-16
Structures of AMP Phosphorylase in a New Carbon Fixation Pathway Reveal its Unique Multimerization and Reaction Mechanism. Yuichi Nishitani, Riku Aono, Takaaki Sato, Haruyuki Atomi, Tadayuki Imanaka, Kunio Miki.

M-17
Fluorescent Methods For Protein Crystallization Screening. Marc Pusey.

M-18
The Key to the Non-Catalytic Domain in Invertases and the Special Case when Mixing High Oligomerization with Low Resolution... the Winding Way! Maria-Angela Sainz-Polo, Beatriz Gonzalez, Alvaro, Maria Fernandez-Lobato, Al Miguel varo Lafraya, Julia Marin, Julio Polaina, Julia Sanz-Aparicio.

M-19
Progress Toward Determining the Structure and Function of the Extra-Cellular Domain of Glucagon Receptor and Complexes with Ligands. Ross Reynolds, Naomi Parker, Li Ren, Augie Pioszak, Eric Xu.

M-20
Crystal Structure of a Zinc-Dependent D-Serine Dehydratase from Chicken Kidney. Toshiya Senda, Miki Senda, Hiroyuki Tanaka, Nagarajan Venugopalan, Atsushi Yamamoto, Tetsuo Ishida, Kihachiro Horiike.

M-21
The Crystal Structure of XPB Helicase from *Pyrobaculum aerophilum*: Implications for the Structure and Mechanism of Human XPB. Michael Sawaya, Sum Chan, Lukasz Goldschmidt, Neil King, Jeanne Perry.

M-22
Structural Characterization of NTDA, a Sugar Aminotransferase Involved in the Production of Kanosamine. Karin van Straaten, Natasha Vetter, David Palmer, David Sanders.

M-23
Structural Analysis of β-Parvin Reveals a Direct Interaction with Paxillin and the Requirements for β-Parvin Localization to Focal Adhesions. Amy L. Stiegler, Kyle M. Draheim, Xiaofeng Li, Naomi E. Chayen, David A. Calderwood, Titus J. Boggon.

M-24
Structure of the Catalytic Chain of *Methanococcus jannaschii* Aspartate Transcarbamoylase in a Hexagonal Crystal Form. Insights into the Path of Carbamoyl Phosphate to the Active Site of the Enzyme. Jacqueline Vitali, Aditya Singh, Alexei Soares, Michael Colaneri.

M-25
Purification and Crystallization of Bacterial Ion-coupled Energizing Protein ExbB. Masahiro Watanabe, Koji Yonekura.

M-26
High-pressure-induced Water Penetration and Pressure Adaptation of IPMDH from Deep-sea Bacteria. Nobuhisa Watanabe, Takayuki Nagae, Yuki Hamajima, Takashi Kawamura, Leonard Chavas, Ken Niwa, Masashi Hasegawa, Chiaki Kato.

M-27
The Worldwide Protein Data Bank: Current Projects. Jasmine Young, Atsushi Nakagawa, Hongyang Yao, Sanchayita Sen.

M-28
Molecular Basis for Genetic Resistance of *Anopheles gambiae* to Plasmodium. Marni Williams, Binh Lee, Shankar Logarajah, Richard Baxter.

M-29
Insights into the Substrate Specificity and Mechanism of the Macrolide Sugar O-Methyltransferase, MycF. Steffen Barnard, David Akey, Shengying Li, David Sherman, Janet Smith.

M-30
Towards a Structural Description of Baeyer-Villiger monooxygenase Substrate Specificity. Brahm J. Yachnin, Peter C.K. Lau, Albert M. Berghuis.

M-31
Biochemical and Biophysical Characterization of the RNA Replication Mechanism of a Small dsRNA Virus. Aaron Collier, Yizhi Tao.

M-32
Bravais General Analysis of Lattices (BGAOL). Herbert Bernstein, Lawrence C. Andrews.

M-33
Structure and Function of Novel Bacterial PLP-dependent Enzymes. Debanu Das, Nicholas Fleischman, Michael Toney, Ashley Deacon, Ian Wilson.

M-34
Why we Need a New Chemical Bond Model. I. David Brown.

M-35
A Possible Mechanism for the Regulation of the PI-PLC from *S. aureus*. Rebecca Goldstein, Jiongjia Cheng, Mary Roberts.

M-36
New Features and How They Work on the D8 QUEST and D8 VENTURE. Garold L. Bryant Jr., Bruce Noll, Michael Ruf.

M-37
Structural Insight into Congenital Sucrase-Isomaltase Deficiency. Kyra Jones, Hassan Y. Naim, David R. Rose.

M-38
Polytypism in the Alkali Tetravalent Metal Trioxides A_2MO_3. Bryan Chakoumakos, Feng Ye.

M-39
Structural Enzymological Studies of Rat Peroxisomal Multifunctional Enzyme, Type-1. Prasad Kasaragod, J. Kalervo Hiltunen, Rik Wierenga.

M-40
The Role of DDLm Methods in Data Validation. Sydney Hall, Nick Spadaccini.

M-41
Broad spectrum ligand binding in biphenyl dehydrogenase (BphBB356): Ternary complex Structures of BphBB356 from *P. pnomenusa*. Pravindra Kumar, Sonali Dhindwal, Dipak Patil.

M-42
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T-06
Structural Implications of an O-methyltransferase from *Planctomyces limnophilus* DSM3776. Norma Duke, Lance Bigelow, Jessica Bearden, Andrzej Joachimiak.

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T-08
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Active site Structure of NDM-1. Youngchang Kim, Christine Tesar, Joy Holowicki, Robert Jedrzejczak, Andrew Binkowski, Gyorgy Babnigg, Joseph Mire, Mark Cunningham, James Sacchettini, Andrzej Joachimiak.

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Approaches to High Throughput Structural Biology Through a Small Lab Experience. Dusan Turk, Marko Mihelic, Andreja Dobersek, Miha Renko, Aleksandra Usenik, Gregor Pretnar.

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2013 Awards:

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Fankuchen	Richard Dickerson
Bau	TBA
Etter Early Career	Eric Ortland

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Deadlines:

Abstracts	March 31
Travel Grants	March 31
Early Registration	May 31
Hotel Conf. rate	July 5

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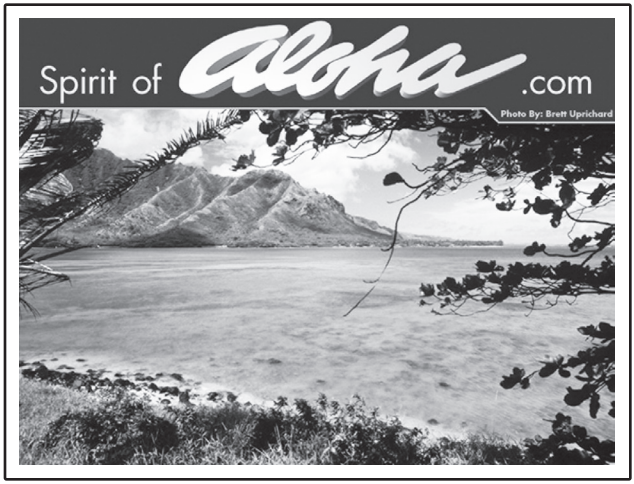

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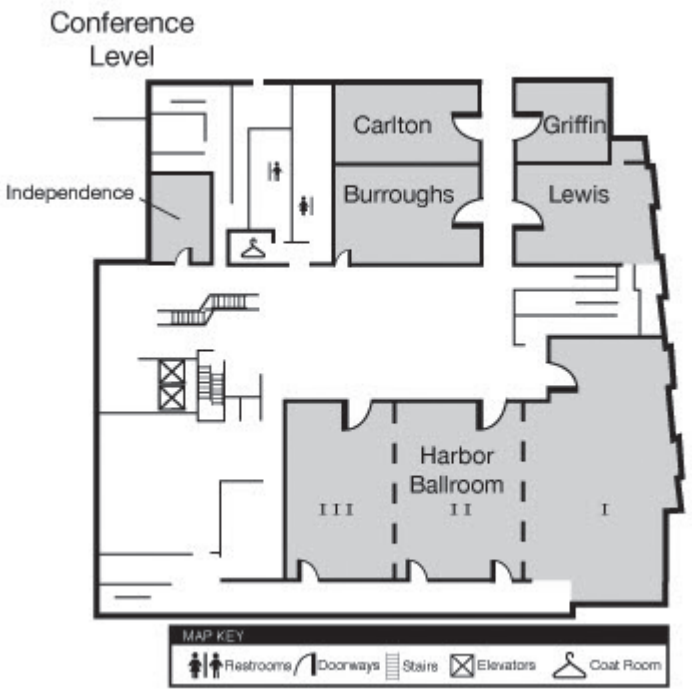

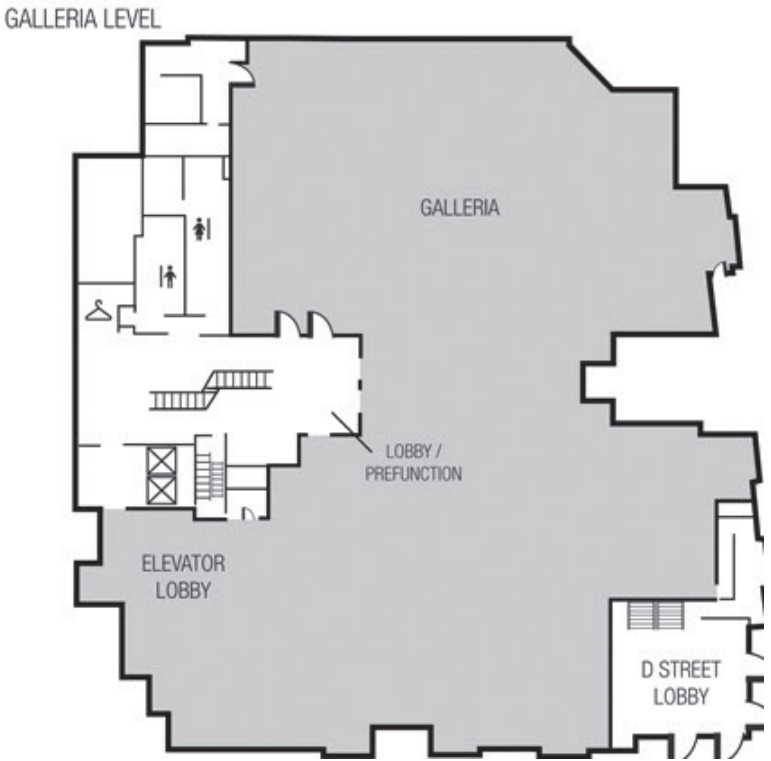

2012 EXHIBIT SHOW Galleria Hall (lower level)

Saturday, 7:30pm-10:30pm Sunday, Monday, Tuesday, 10:00am-7:30pm

EXHIBITORS

Agilent Technologies .....#430
Anton Paar.....#330
Area Detector Systems Corp.....#327
Art Robbins Instruments .....#411
Australian Synchrotron.....#334
Blake Industries, Inc. .....#410
Bruker AXS, Inc. .....#321, 325
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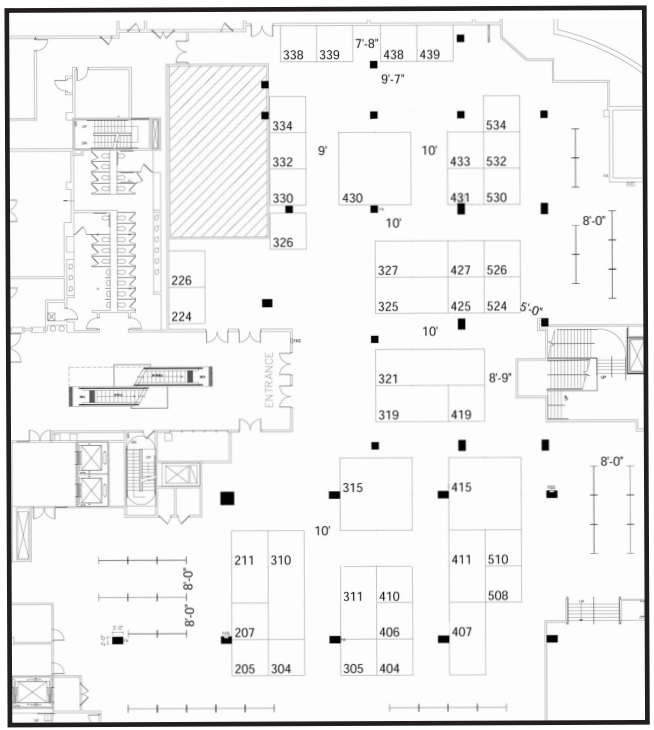

Program at a Glance

Saturday July 28

Morning

WK.01 Refmac and Coot — Harbor I
IWK.02 OLEX2 — Harbor II
WK.03 Modeling & Refinement of Nanoparticle Structures from Diffraction Data — Lewis
WK.04 Crystallography - World of Wonders — Burroughs

Afternoon

WK.01 Refmac and Coot — Harbor I
WK.02 OLEX2 — Harbor II
WK.03 Modeling & Refinement of Nanoparticle Structures from Diffraction Data — Lewis
WK.04 Crystallography - World of Wonders — Burroughs

Evening

New Attendee/Student Orientation 5:30pm — Lewis
SP.01 Innovations in Undergraduate Education
Eric Mazur 6:30pm — Harbor II
Opening Reception, Presidential Welcome and Exhibit Show 7:30pm — Galleria Hall

Sunday July 29

Morning

AW.01 ACA Buerger Award to John Spence — Harbor I
TR.01 Transformations and Structural Oddities in Molecular Crystals: In Honor of Bruce Foxman — Harbor I
01.01 Structural Genomics for the Home Lab — Harbor III
09.01 Functional Nanomaterials — Lewis
13.01 Emerging Sources: Theory and Practice I — Burroughs
13.02 Magnetic Materials — Harbor II

Afternoon

SIG Meetings:
Canadian Division, General Interest, Syn Radiation 12:00-12:30pm
BioMac, Small Angle Scattering 1:00-1:30pm

Rigaku Lunch — Stone

TR.01 Transformations and Structural Oddities in Molecular Crystals: In Honor of Bruce Foxman — Harbor I
03.01 General Interest I — Lewis
13.03 Fibril-Forming Pathological — Harbor II
01.02 Structural Approaches to Enzyme Mechanisms — Harbor III
13.04 Emerging Sources: Theory and Practice II — Burroughs

Evening

Poster Session S 5:30pm — Galleria Hall
YSSIG Mixer (ticket required) 8:00pm — Harbor II

Monday July 30

Morning

AW.02 ACA Warren Award to Paul Fenter — Harbor I
13.05 Emerging Sources: Theory and Practice III — Burroughs
09.02 Macromolecular Science with Scattering Methods — Lewis
13.06 Materials for a Sustainable Future I — Harbor II
13.07 Reflections & Future Directions: 100 Yrs of Diffraction — Harbor III
13.08 Exciting Structures — Harbor I

Afternoon

SIG Meetings:
Fiber Diffraction, Industrial, Joint Service & Sm Mol 12:00-12:30pm
Joint Neutron/Materials/Powder, Young Scientists 1:00- 1:30pm

Agilent Lunch
Bruker Lunch — Otis

13.09 Protein & Small Molecule Cr @ Undergrad Inst. — Lewis
13.10 Radiation Damage — Harbor I
01.03 Structural Enzymology—Biology — Harbor III
13.06 Materials for a Sustainable Future II — Harbor II
13.11 Flesh & Blood: Tissue Diffraction Studies — Burroughs

Evening

Poster Session M 5:30pm — Galleria Hall

Tuesday July 31

Morning

AW.03 Etter Early Career Award to Emmanuel Skordalakes — Harbor I
12.01 Etter Early Career Award Symposium — Harbor I
13.12 Complementary Methods in Structural Biology: Spectroscopy, Microscopy and Others — Harbor III
10.01 Important Science From Small Molecule Structures — Harbor II
13.13 Total Scattering Analysis — Lewis
09.04 Precipitates and Voids in Advanced Materials — Burroughs

Afternoon

09.05 Complementary Techniques in Structural Biology — Burroughs
10.02 Cool Structures — Harbor II
13.14 Extended Wavelength X-ray Crystallography — Harbor I
13.15 *In operando/in situ*/Parametric Studies — Lewis
13.16 From Constructs to Crystals — Harbor III
ACA Member's Business Meeting 5:00pm (all are welcome) — Harbor II

Evening

Poster Session T 5:30pm — Galleria Hall
08.01 Would you Publish This? 7:00pm — Burroughs

Wednesday August 1

Morning

AW.04 Supper Award to Ron Hamlin — Harbor I
TR.01 Transformations and Structural Oddities in Molecular Crystals: In Honor of Bruce Foxman — Harbor I
11.01 Advanced Hardware and Applications — Burroughs
13.18 Public Domain Software — Harbor II
13.19 Functional and Emerging Materials & Technology — Lewis
13.20 Membrane Proteins from Start to Finish — Harbor III

Afternoon

03.02 General Interest II — Burroughs
13.21 Crystallographic Information in Pharma R&D — Harbor II
13.22 Structure-Guided Drug Discovery — Harbor III
13.23 Data Collection with the Pros — Harbor I
13.24 Phase Transitions in Inorganic Systems — Lewis

Evening

SP.02 The History of Structural Biology
Donald Caspar 5:15pm — Harbor II

Annual Awards Banquet — Harbor II & III
(ticket required) Cash Bar 6:30pm Dinner 7:30pm

Thursday August 2

Planning Session for 2013 ACA Annual Meeting in Honolulu, Hawaii, July 20 - 24, 2013 — Burroughs

2012 EXHIBIT SHOW Galleria Hall (lower level)
Saturday, 7:30pm-10:30pm Sunday, Monday, Tuesday, 10:00am-7:30pm

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