

American Crystallographic Association Annual Meeting July 20 - July 24, 2013, Honolulu, HI

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Poster Chair: Ilia Guzei

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SATURDAY, JULY 20

WK.01 Biological Small Angle Solution Scattering - Theory and Practice

Organizers: Richard Gillilan (MacCHESS, Cornell Univ.), Edward Snell (Hauptman-Woodward Medical Research Institute)

Track A: Honolulu/Kahuku

Track B: Oahu/Waialua

Small angle solution scattering (SAS) is experiencing a dramatic increase in popularity within the structural biology community. The availability of synchrotron radiation and neutron sources, commercial lab-source SAXS instrumentation, low-noise detectors, powerful computing hardware, and better algorithms, has made the technique accessible to a much larger audience than ever before. At the same time, biologists are investigating ever more complex systems that pose increasing challenges to conventional crystallography. Given that 75% to 80% of soluble, purified, protein samples fail to crystallize, having a solution-based technique that can provide some structural information is compelling. In addition, biological systems are studied more and more in the context of biologically relevant multi-macromolecule complexes. SAS is an excellent technique to pursue these problems.

This dual-track workshop brings together leading beamline scientists, experts in laboratory-based BioSAXS sources, and experienced users of the technique, to provide a unique, practical, "HOW TO" course in SAS data collection, processing, and interpretation. While a single day of lectures and computer exercises can hardly begin to cover the many powerful aspects of solution scattering, this course is designed to provide a foundation of essential information for any serious student wishing to apply SAS methods to problems in biology. Students will additionally have the opportunity to interact with experts to plan their proposed experiments.

Organizing committee: Michal Hammel (Advanced Light Source), Thomas Irving (Advanced Photon Source), Lin Yang (National Synchrotron Light Source), Thomas Weiss

(Stanford Synchrotron Light Source), Mark van der Woerd (Colorado State University), Matthew Benning (Bruker AXS), Gerd Langenbacher (Anton-Paar), Angela Criswell (Rigaku)

Workshop sponsors: Bruker, Rigaku, Anton Paar, Wyatt Technology, Incoatec, and Dectris

Track A: Getting Started in Biological Small Angle Solution Scattering: Your practical HOW TO Guide

The "Beginners Track" will focus on basic essentials and presumes that students have little or no previous SAS knowledge. The sessions will include both lectures and practical computer exercises. Emphasis will be placed on basic requirements for acceptable publication of SAS data. Topics also include sample preparation and guidelines for judging data quality, what to do about problematic (aggregated) samples, Guinier analysis, molecular weight determination, inverse Fourier methods and envelope calculations. Students will also learn some basics for home laboratory data collection and receive information about the various synchrotron BioSAXS beamlines. While this workshop is primarily focused on biological X-ray solution scattering, we expect to provide some content to raise student awareness on the unique opportunities and advantages presented by neutron scattering.

Speakers:

Angela Criswell (Rigaku), Javier Perez (Soleil), Srinivas Chakravarthy (APS), Jill Trehwella (U. Sydney), Richard Gillilan (MacCHESS, Cornell U.), Andreas Keilbach (Anton Paar), Juergen Graf (Incoatec), Edward Snell (HWI).

8:00 am Registration and software installation help, introduce speakers

8:30 am BioSAS Welcome and Overview

8:45 am Basics: Scattering profile, Guinier analysis, monodispersity, etc.

9:15 am Tutorial 1: Good data vs. bad data, tell the difference, identify problems

10:15 am Coffee Break

10:30 am Molecular weight, Kratky plot &

flexibility, $P(r)$ function

11:00 am Tutorial 2: Calculate a $P(r)$ function, determine MolWt, D_{max} , R_g , $I(0)$

12:00 pm Lunch (provided)

1:00 pm Sample preparation: I have aggregation, now what?

1:30 pm Shape reconstruction: how much can you believe?

2:00 pm Tutorial 3: Shape reconstruction HOW TO

3:00 pm Coffee break

3:15 pm Do try this at home: home source data collection

4:15 pm Going beyond SAXS with SANS

5:00 pm Publishing your first SAS data: what you should know

5:30 pm Conclusion

Track B: Using Advanced Methods in Biological Small Angle Solution Scattering

The parallel “Advanced Methods Track” will cater to the needs of the growing pool of experienced BioSAXS users who have mastered basic SAS data collection and analysis and are ready to tackle more advanced analytical processing techniques. The session will focus on tools and proper techniques for evaluating SAXS data, molecular mass, and flexibility. Modeling software: FOXS, MES, FoxDOCK, AllosMod-FOXS. Topics also include inference-free data, similarity maps, heavy atom labeling, ensemble analysis, mixtures and size exclusion chromatography, NMR+SAXS, *ab initio* modeling at the residue level. Since many departments and multi-college consortia are starting to think about building lab-based BioSAXS facilities, a special lecture is planned which will help familiarize students with the various approaches and potential challenges for building lab source BioSAXS facilities.

Speakers: Robert Rambo, Michal Hammel, Greg Hura (ALS), Kushol Gupta (Perelman School of Medicine, U. Penn), Alexander Grishaev (NIH/NIDDK), Emre Brookes (U. Texas Health Sci Center), Andreas Keilbach (Anton Paar), Juergen Graf (Incoatec), Angela Criswell (Rigaku), and others.

8:00 am Registration and software installation help, introduce speakers

8:30 am Criteria for evaluation of SAXS data-part 1.

9:45 am Criteria for evaluation of SAXS data-part 2.

10:15 am Coffee break

10:30 am Tutorial 1: Practical session with SCATTER, FOXS, MES, FOXSDOCK and SSM

12:00 pm Lunch (provided)

1:00 pm Contrast Matched SAXS from a Heavy Atom Labeled Protein

1:45 pm SAXS combined with crystallography and computation: Application of the Ensemble Analysis, SASSIE

2:30 pm Advanced techniques in using crystallography, NMR and SAXS to model solution structure

3:00 pm Mixtures: HPLC+SAXS, US-SOMO software

3:15 pm Coffee break

3:30 pm Tutorial 2: Solution structure modeling: Computational techniques for modeling macromolecular flexibility, Ensemble modeling, *ab initio* modeling at the residue level etc.

4:30 pm Building a BioSAXS Lab Source: things you should know

5:30 pm Conclusion

SATURDAY, JULY 20

WK.02 GSAS-II Workshop

Organizers & Instructors: Brian Toby and Robert Von Dreele
Waianae

The workshop will introduce the attendees to the use of the new GSAS-II software package for the reduction, solution and refinement of crystallographic data, with particular emphasis on powder diffraction data. All software needed to install and run the software is freely available. The workshop will be targeted toward individuals with some experience with Rietveld analysis and to experienced single-crystal crystallographers with some knowledge of powder diffraction. Attendees are required to bring their own laptops with the software already downloaded. Installation instructions are found at <http://subversion.xray.aps.anl.gov/trac/pyGSAS>.

The GSAS-II software suite will be the eventual replacement for GSAS and its associated graphical user interface (GUI) package, EXPGUI, which are likely the most widely used crystallography software package for materials crystallography, particularly for neutron and synchrotron powder diffraction (Rietveld) fitting, but GSAS also sees use for neutron single-crystal analysis and combined x-ray single crystal/neutron powder diffraction analysis. As one measure of their importance, GSAS and EXPGUI together have received >7,000 citations and continue to be cited many hundreds of times annually.

The GSAS-II package has much wider goals than GSAS. Although over time its capabilities will continue to advance, the GSAS-II package already has capabilities needed for all aspects of powder diffraction crystallographic analysis, including area detector data reduction, indexing, and structure solution by charge flipping, in addition to the refinement and Fourier map analysis capabilities that duplicate GSAS features. GSAS-II can be used for analysis of constant-wavelength x-ray and neutron powder data, as well as X-ray and neutron single-crystal data. Oak Ridge National Laboratory has indi-

cated an interest in driving the adaptation for time-of-flight neutrons. GSAS-II is a completely modern code, written almost completely in Python and designed with a sophisticated GUI and with advanced visualization features integrated. GSAS-II is open source and is freely distributed. GSAS-II has recently been made available to the public, with the understanding that new capabilities are being added and bugs addressed on a continuing basis.

Because GSAS-II includes an area detector calibration and integration module, the software may be of interest within the APS where powder diffraction is used for calibration of area detector placement, or where radial integration is used.

The workshop will concentrate on use of GSAS-II for powder diffraction and will cover reduction of area detector powder diffracton images, structure solution and Rietveld structure refinement techniques. Attendees should bring their own laptops (Windows, Mac and Linux are all supported) and should install GSAS-II prior to the workshop. Help will be provided at the workshop to install the software for anyone who has had trouble.

- 8:00 Coffee, tea and solving software installation problems
- 9:00 An overview of GSAS-II capabilities
- 9:45 Area detector data reduction demo
- 10:00 Coffee break
- 10:20 Self-paced exercise 1: Area detector data calibration and reduction
- 11:00 Autoindexing, charge-flipping and Fourier demo
- 11:20 Self-paced exercise 2: Autoindexing, structure solution & completion
- 12:00 Lunch break
- 1:30 Self-paced exercise 2, continued
- 2:15 Introduction to GSAS-II refinement capabilities and Rietveld demo
- 2:45 Self-paced exercise 3: Rietveld refinement exercise
- 3:30 Coffee break
- 3:50 Overview of restraints and constraints
- 4:10 Planned future developments for GSAS-II
- 4:30 Participant feedback on potential

SATURDAY, JULY 20

WK.03 Get the Most out of the Cambridge Structural Database System

Organizer & Instructor: Pete Wood, (CSD)

Instructor: Colin Groom (CSD)

Kohala/Kona

The Cambridge Structural Database (CSD) is the world's repository for small molecule organic and metal-organic crystal structures. As such, this chemically diverse database of more than 600,000 molecules is a crucially important resource for pharmaceutical discovery, materials development, research and education. The Cambridge Crystallographic Data Centre (CCDC) not only distribute the CSD but also provide a comprehensive set of software tools that enable the valuable structural data to be searched, analysed, visualised and explored.

This workshop will introduce you to the database and its associated software, known collectively as the CSD System, and illustrate the use of these structural data in a variety of applications. The workshop is ideal for inexperienced and experienced users alike and will feature introductory presentations for each component of the CSD System followed by the opportunity to use the software hands-on guided by our illustrative tutorials. Our experienced staff will be available to assist with any questions you might have. At the end of the workshop there will be the opportunity to learn more about WebCSD or to trouble-shoot with our experienced tutors.

09:00 Introduction to the CCDC and the CSD System: ConQuest, Mercury and Data Analysis Tools (Colin Groom)

09:30 Hands-on Session 1: Using ConQuest, Mercury and Data Analysis Tools (Colin Groom, Pete Wood)

10:30 Coffee break

11:00 Introduction to the CSDS continued: Advanced Mercury Functionality and Solid Form Suite (Pete Wood)

11:30 Hands-on Session 2: Using Advanced Mercury Functionality and Solid Form Suite (Colin Groom and Pete Wood)

12:30 Lunch (provided)

1:30 Introduction to the CSDS continued: Mogul and IsoStar

2:00 Hands-on Session 3: Using Mogul and IsoStar (Colin Groom and Pete Wood)

3:00 Coffee break

3:30 Introduction to WebCSD, the Online Search Interface to the CSD (Pete Wood)

4:00 Choice of Hands-on Session 4: WebCSD or Question and Answer Session

Saturday Evening Activities

First Time Attendee and Student Meeting Orientation

5:30pm Kohala/Kona

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

Opening Reception and Exhibit Show

7:30pm Ballroom

Must have meeting name badge for entry

SUNDAY, JULY 21

Registration Desk.....	07:30am.....	Ballroom Foyer
Speaker Ready Room.....	07:30am.....	lao Needle
Council Meeting Room	07:30am.....	Puna
Exhibit Show.....	10:00am.....	Ballroom
Rigaku Lunch & Learn	12:00pm.....	Royal Hawaiian Hotel-Regency Room III (invitation only pick up ticket at Rigaku booth)
Fiber Diffraction SIG Meeting	12:00pm.....	Kohala/Kona

AW.01 Robert Bau Award Presentation and Lecture

Cheryl Stevens, presiding

Lanai

08:00-08:45am AW.01.01

From the Amino Acid Structures to Metal Hydrides: Four Decades of Single-Crystal Neutron Diffraction. Thomas Koetzle.

11.01 Multi-crystal and Micro-crystal Data Collection

John Rose, Marian Szebenyi, presiding

Kohala/Kona

Funding for this session provided, in part, by Cornell Univ.-
Cornell High Energy Synchrotron Source

09:00-09:20am 11.01.01

Microfluidics for Nucleation Rates and *in situ* X-Ray Diffraction of Protein Crystals. Seth Fraden, Michael Heymann, Sathish Akella, Achini Opathalage.

09:20-09:40am 11.01.02

Integration of *in situ* X-ray Diffraction Analysis with High-throughput Crystallization Screening. Rick Roberts, Robin Owen, Joseph Luft, Gaetano Montelione, Edward Snell.

09:40-10:00am 11.01.03

The Protein Micro-crystallography at SPring-8. Masaki Yamamoto, Kunio Hirata, Yoshiaki Kawano, Go Ueno, Hironori Murakami, Takaaki Hikima, Takashi Kumasaka.

10:00-10:30am Coffee Break

10:30-10:50am 11.01.04

Graphene as a Mounting Material for Protein Crystals. Jennifer Wierman, Jonathan Alden, Paul McEuen, Sol Gruner.

10:50-11:10am 11.01.05

Synchrotron-based Multi-crystal Crystallography. Qun Liu, Yanqi Chang, Youzhong Guo, Zahra Assur, Filippo Mancina, Wayne Hendrickson.

11:10-11:35am 11.01.06

Improvement of Data Quality for Radiation Sensitive Crystals Using Multi-Crystal Diffraction Assembly Methods. Michael Hanson, Gye Won Han, Michael Sawaya, Mauro Mileni, Jill Chrencik, Vadim Cherezov, Peter Kuhn, Raymond Stevens.

11:35-12:00m 11.01.07

Novel Procedures to Obtain Structure from Microcrystals. Sol M. Gruner.

13.01 Structural Enzymology (I)

Gerald Audette, Rebecca Page, presiding

Lanai

Funding for this session provided, in part, by Art Robbins
Instruments, Molecular Dimensions, Rigaku Americas

09:00-09:05am

Welcome and Thanks to Sponsors

09:05-09:30am 13.01.01

The Mega-Synthases from Polyketide and Fatty Acid Biosynthetic Pathways. Sheryl Tsai.

09:30-09:45am 13.01.02

Structural Studies of the Aminoglycoside Kinase APH(2'')-IVa and its Inhibitors. Kun Shi, Albert Berghuis.

09:45-10:00am 13.01.03

Eliminating Drug-Induced GI Toxicity by Potently Disrupting a Symbiotic Bacterial Enzyme. Adam Roberts, Bret Wallace, Madhu Venkatesh, Urs Boelsterli, Sridhar Mani, Matthew Redinbo.

Small Angle Scattering SIG Meeting	12:00pm.....	Honolulu/Kahuku
Joint SIG Meeting: Service & Small Molecules	12:00pm.....	Waianae
BioMac SIG Meeting	5:00pm.....	Lanai
GIG SIG Meeting	5:00pm.....	Honolulu/Kahuku
Poster Session S	5:30pm - 7:30pm	Ballroom
YSSIG Mixer (ticket required).....	8:00pm.....	Princess Kaiulani Hotel, Kapuni Room

10:00-10:30am Coffee Break

10:30-10:55am 13.01.04
 Structure-based Analysis and Inhibition of Cell-wall Biogenesis in Pathogenic Bacteria. Natalie Strynadka.

10:55-11:10am 13.01.05
 Multifaceted Analysis of PA4794 - A New Protein Acetyltransferase. Karolina Majorek, Misty Kuhn, Maksymilian Chruszcz, Wayne Anderson, Wladek Minor.

11:10-11:35am 13.01.06
 Protein Phosphatases: Structural Basis For Function And Specificity. Wolfgang Peti, Meng Choy, Senthil Kumar, Simina Grigoriu, Clarissa Eibl, Manuel Hessenberger.

11:35-12:00pm 13.01.07
 Mechanisms of Activation and Inhibition of the Ubiquitin Conjugating Enzyme, Ubc13. Mark Glover, Curtis Hodge, Stephen Campbell, Jiyong Zhao.

13.02 Nanomaterial Structure from Diffraction Data (I): Theory and Modeling

Katharine Page, presiding
Oahu/Waialua

09:00-09:30am 13.02.01
 Implicit Assumptions about Spatial Dimensions in Diffraction Analysis. Ismail C. Noyan, Hande Ozturk, Hanfei Yan, John R. Hill.

09:30-10:00am 13.02.02
 Pair Distribution Function Study of the Nanostructured Mo-V-(Nb/Te) Oxides. Tatyana Kardash, Ludmila Plyasova, Valentina Bondareva, Reinhard Neder.

10:00-10:30am Coffee Break

10:30-11:00am 13.02.03
 Coherent X-ray Diffraction Imaging from Nanostructures. Edwin Fohtung, Jong Woo, Ross Harder, Na Le, Phillippe Lecoeur, Dafine Ravelosona, Eric Fullerton, Oleg Shpyrko.

11:00-11:30am 13.02.04
 Simulation of Short Ranged Ordered Decorated Nanoparticles. Reinhard Neder.

11:30-12:00pm 13.02.05
 Local Symmetry Increase on Cooling in KNi_2Se_2 : Representational Analysis of Extended Disorder in Large Atomistic Ensembles. Tyrel McQueen, James Neilson.

13.03 Improving Structural Models through Computational Tips & Tricks

Louise Dawe, Jason Mercer, presiding
Waianae

09:00-09:30am 13.03.01
 The Squeeze Tool in Platon and its Use With Shelx12013 L.S. Refinement. Anthony Spek.

09:30-09:50am 13.03.02
 CrowdPhase: Crowdsourcing the Phase Problem. Julien Jorda, Todd Yeates.

09:50-10:30am Coffee Break

10:30-11:00am 13.03.03
 Who is Afraid of a Pseudo-Merohedral Twin? Ilia Guzei, Regine Herbst-Irmer, Apollinaire Munyaneza, James Darkwa.

11:00-11:20am 13.03.04
 Score Maps Improve the Clarity of Density Maps. Dusan Turk.

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11:20-11:40am **13.03.05**
Crystallography and Molecular Modeling: A Co-Dependent Relationship. Amy Sarjeant, Robert Kennedy, Daniel Clingerman.

11:40-12:00pm **13.03.06**
How to Decrease R-free? Zbyszek Otwinowski, Dominika Borek, Marta Orlikowska, Stephan Ginell, Wladek Minor, Marcin Cymborowski, Przemyslaw Porebski.

TR.01 Transactions Symposium Neutron & Synchrotron Sources: Role in Crystallography (I): Small Angle Scattering

Richard Gillilan, Greg Hura, presiding
Honolulu/Kahuku

09:00-09:30am **TR.01.01**
High-throughput SAXS as a Complement to Crystallography. Edward Snell, Thomas Grant, Joseph Luft, Thomas Weiss, Tsutomu Matsui, Lester Carter.

09:30-09:45am **TR.01.02**
FPLC-coupled SAXS: Potential Strategy for Enhancing Sample Homogeneity and Data Quality. Srinivas Chakravarthy, Thomas Irving.

09:45-10:00am **TR.01.03**
Connecting Structure with Biology by Combining SAXS and Crystallography. Greg Hura, Kevin Dyer, Michal Hammel, Robert Rambo, David Shin, John Tainer.

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

10:30-11:00am **TR.01.04**
Using SAXS to Monitor Aggregation Propensities of Amyotrophic Lateral Sclerosis Mutants of Superoxide Dismutase. Ashley Pratt, David Shin, Gregory Merz, W. Andrew Lancaster, Kevin Dyer, Peter Borbat, Michael Adams, Jack Freed, Elizabeth Getzoff, John Tainer.

11:00-11:15am **TR.01.05**
Automation and High-throughput SAXS Approaches at the Bio-SAXS/D Beamline BL4-2 at SSRL. Thomas Weiss, Tsutomu Matsui, Lester Carter, Ping Liu.

11:15-11:45am **TR.01.06**
Biological SAXS at the Australian Synchrotron. Nigel Kirby, Simone Beckham, Stephen Mudie, Adrian Hawley, Haydyn Mertens, Nathan Cowieson, Vesna Samardzic-Boban, Matthew Wilce, Ulrich Felzmann, Jack Dwyer, Joanna Huang, Jarrod Sinclair, Andreas Moll.

11:45-12:00pm **TR.01.07**
Chips and Robots: Screening, Mixing, and Dialysis on BioSAXS Beamlines. Richard Gillilan, Mike Cook, Gregori Temnykh, Magda Møller, Søren Nielsen.

03.01 General Interest (I)

Xiaoping Wang, presiding
Honolulu/Kahuku

01:30-01:50pm **03.01.01**
Processing of Shutterless CMOS Detector Data with the Bruker Apex2 Software Suite. Charles Campana, Joerg Kaercher, Greg Wachter, Stephen Leo, Bruce Noll.

01:50-02:10pm **03.01.02**
The Pilatus 200K Detector for Small-Molecule Crystallography. Lee Daniels, Joseph Ferrara, Masataka Maeyama, Mark Pressprich.

02:10-02:30pm **03.01.03**
Better Data Quality and Advances in Twin Data Processing in CrysAlisPro. Mathias Meyer.

02:30-02:50pm **03.01.04**
Beam Conditioning in Cutting Edge X-ray Analytical Equipment. Juergen Graf, Andreas Kleine, Carsten Michaelsen, Christoph Ollinger.

02:50-03:30pm **Coffee Break**

03:30-03:50pm **03.01.05**

Current Status of the Liquid-Metal-Jet X-ray Source Technology. Bjorn Hansson, Oscar Hemberg, Mikael Otendal, Tomi Tuohimaa, Per Takman.

03:50-04:10pm **03.01.06**

Improving Light-Atom Absolute Configuration Determination with Ga K α Wavelength. Michael Ruf, Garold L. Bryant, Jr., Bruce C. Noll.

04:10-04:30pm **03.01.07**

The Compact Light Source - a New Generation Synchrotron X-ray Source. Roderick Loewen, Ronald Ruth.

04:30-04:50pm **03.01.08**

Neutron Scattering under High Pressure: SNAP - Recent Results and Future Directions. Antonio M. dos Santos, Jamie J. Molaison, Christopher A. Tulk.

09.01 Dynamic & Flexible Structures in Biomolecules (I)

Yun-Xing Wang, presiding

Waianae

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

01:30-02:00pm **09.01.01**

Quantitative Analyses of Unstructured and Flexible Complexes Plus Comprehensive Conformational Maps from Biological Small Angle X-Ray Scattering With Crystallography. John Tainer, Robert Rambo, Greg Hura, Michal Hammel.

02:00-02:30pm **09.01.02**

Dynamics and Kinetics of the Aptamer Domain of Adenine Riboswitch RNA for Ligand Uptake. Xiaobing Zuo.

02:30-03:00pm **09.01.03**

Plasma Lipoproteins: Where Flexibility and Dynamics is at the Heart of Biological Function. Peter Laggner, Ruth Prassl, Matthew Benning.

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

03:30-03:45pm **09.01.04**

Intramolecular SH3-PRD Domain Interactions Underlie the Molecular Basis for Calcium-Dependent Conformational Changes in Rat Endophilin A2. Kushol Gupta, Miao Zhang, Yuan Chen, Patrick Loll, Gregory Van Duynes, Ji-Fang Zhang.

03:45-04:00pm **09.01.05**

Solution Structure of the IL-33 Signaling Complex. Shu-Ying Wang, Xi Liu, Michal Hammel, Xinquan Wang.

04:00-04:15pm **09.01.06**

Investigation of Phonon-like Excitation in Hydrated Protein Powders by Neutron Scattering. Xiang-qiang (Rosie) Chu, Eugene Mamontov, Hugh O'Neill, Qiu Zhang, Alexander Kolesnikov.

04:15-04:30pm **09.01.07**

Super-resolution in Solution X-ray Scattering and its Applications to Structural Systems Biology. Robert Rambo, John Tainer.

04:30-04:15pm **09.01.16**

Solution Structure and Biochemical Characterizations of a Designed Tandem Coiled Coil Protein. Donghyuk Shin, Gwanho Kim, Yang-Gyun Kim, Sangho Lee.

11.02 Femtosecond X-ray Pulses: Tools for Crystallography

Michael Bogan, presiding

Kohala/Kona

01:30-02:00pm **11.02.01**

Recent Nano Crystallography Experiments at CXI. Marc Messerschmidt, Sebastien Boutet, Garth Williams.

02:00-02:30pm **11.02.02**

2D Protein Crystallography using XFELs: Results, Challenges, and Potential Solutions. Mark Hunter, Matthew Coleman, James Evans, Nadia Zatspein, Stefan Hau-Riege, Ch-

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ing-Ju Tsai, Xiaodan Li, Bill Pedrini, Gebhard Schertler, Matthias Frank.

02:30-03:00pm 11.02.03

Femtosecond High-resolution Diffraction Studies of Metalloproteins at LCLS. Aina Cohen, Winnie Bremmer, Ying Chen, Henrik Lemke, James Holton, Jinhu Song, S. Michael Soltis, C. David Stout, Yingsu Tsai, Diling Zhu.

03:00-03:30pm Coffee Break

03:30-04:00pm 11.02.04

XFEL Data Processing with cctbx.xfel. Johan Hattne, Aaron Brewster, Nathaniel Echols, Richard Gildea, Nicholas Sauter.

04:00-04:30pm 11.02.05

Simultaneous INverse Beam Anomalous Diffraction (SINBAD). James Holton, Alastair MacDowell, John Spence.

13.04 Nanomaterial Structure from Diffraction Data (II): Experimental Advances

Katharine Page, presiding

Oahu/Waialua

01:30-02:00pm 13.04.01

Methodological and Software Advances for Nanostructure Science. Simon Billinge.

02:00-02:30pm 13.04.02

Structure and Dynamics of the Surface Water on SnO₂ Nanocrystals. Hsiu-Wen Wang, David Wesolowski, Thomas Proffen, Lukas Vlicek, Alexander Kolesnikov, Wei Wang, Jorge Sofo, James Kubicki, Paul Kent, Lawrence Anovitz.

02:30-03:00pm 13.04.03

Pulsed-reactant *in situ* Studies of "Inverse" Cu/ceria Catalysts using Simultaneous XRD and DRIFTS Measurements. Jonathan Hanson, R. Si, W. Xu, S.D. Senanayake, K. Mudiyanselage, J. Rodriguez, E. Dooryhee, A. Yakovenko, K. Chapman, P. Chupas.

03:00-03:30pm Coffee Break

03:30-04:00pm 13.04.04

Understanding Hydrogen Storage Properties of Materials from the Local Structure. Hyun-jeong Kim.

04:00-04:20pm 13.04.06

Evolution of Crystalline Order in ZnO Nanoparticles in Sub-nanometer Range via *in-situ* PDF. Mirijam Zobel, Reinhard B. Neder.

TR.02 Transactions Symposium Neutron & Synchrotron Sources: Role in Crystallography (II): Supramolecular Assemblies

Christine Dunham, Eric Montemayor, presiding Lanai

Funding for this session provided, in part, by Art Robbins Instruments, DECTRIS, Emerald Biosystems, Fisher Scientific, Formulatrix, Hampton Research Corp., MiTeGen, Molecular Dimensions

01:30-02:00pm TR.02.01

Structural Studies of Ribosome-Dependent Toxins Active During the Stringent Response. Christine Dunham, Marc Schureck, Tatsuya Maehigashi, Jack Dunkle, Stacey Miles, Jhomas Marquez.

02:00-02:30pm TR.02.02

The Active Site and Evolutionary Origin of the Spliceosome. Kiyoshi Nagai, Wojciech Galej, Thi Hoang Duong Nguyen, Chris Oubridge, Jade Li, Andy Newman.

02:30-03:00pm TR.02.03

Structure Studies of Ribonucleoprotein Particles in CRISPR Pathways. Hong Li.

03:00-03:30pm Coffee Break

03:30-04:00pm TR.02.04

Molecular Mechanisms of PLC β Activation. Angeline Lyon, Somnath Dutta, Cassandra Boguth, Georgios Skiniotis, John Tesmer.

SUNDAY, JULY 21

04:00-04:30pm

TR.02.05

Structural Studies of Bacterial Transcription Complexes. Seth Darst, Brian Bae, Elizabeth Campbell, Elizabeth Davis, Andrey Feklistov, Jesse Hauver, Elizabeth Hubin, Katherine Leon, Natacha Opalka, Albert Weixlbaumer.

04:30-05:00pm

TR.02.06

Damaged DNA Induced UV-damaged DNA-Binding Protein (UV-DDB) Dimerization and its Roles in Chromatinized DNA Repair. Joanne Yeh, Arthur Levine, Shoucheng Du, Unmesh Chinte, Harshad Ghodke, Hong Wang, Haibin Shi, Vesna Ropic-Otrin, James Conway, Bennett Van Houten.

12.01 Career Odyssey Panel

**Katherine Hicks, Megan Sikowitz, presiding
Oahu/Waialua**

05:00-06:30pm

Heba Abourahma, The College of New Jersey

James Holton, Lawrence Berkeley National Laboratory

Michael Hanson, Receptos, Inc.

Rebecca Page, Brown University

Zoe Fisher, Los Alamos National Laboratory

Jim Pflugrath, Rigaku

2013 Margaret C. Etter Student Lecturer Awards

Each Scientific 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 SIG. 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.....	Adam Roberts, UNC - Chapel Hill	13.01.03
General Interest.....	Colleen Lopez, California State Univ. San Marcos.....	03.02.04
Materials Science.....	Mirijam Zobel, Univ. Erlangen, Germany.....	13.04.06
Neutron Scattering.....	Rebecca Beadling, Indiana Univ. of Pennsylvania.....	13.18.03
Service Crystallography	Christopher Rackauckas, Oberlin College	13.06.10
Small Angle Scattering.....	Donghyuk Shin , Sungkyunkwan Univ., Korea	09.01.16
Small Molecule	Andrew Cairns, Univ. of Oxford, UK.....	13.06.08
Synchrotron Radiation	Jennifer Wierman, Cornell Univ.....	11.01.04
Young Scientist.....	Karim Sutton, Univ. of Oxford, UK	12.02.07

MONDAY, JULY 22

Rigaku Fun Run.....	6:00am.....	Sheraton Hotel Lobby
Registration Desk.....	07:30am.....	Ballroom Foyer
Speaker Ready Room.....	07:30am.....	lao Needle
Council Meeting Room.....	07:30am.....	Puna
Exhibit Show.....	10:00am.....	Ballroom
DECTRIS Lunchtime Seminar.....	12:00pm.....	Royal Hawaiian Hotel-Regency Room III
Young Scientists SIG Meeting.....	12:00pm.....	Lanai

AW.02 Fankuchen Award Presentation and Lecture

Cheryl Stevens, presiding

Lanai

08:00-08:45am AW.02.01

Richard E. Dickerson: A Retrospective. Alex McPherson.

09.02 Nanostructured Thin Films - Frontiers of Grazing Incidence Scattering

Hiroshu Okuda, Detlef Smligies, presiding

Waianae

09:00-09:30am 09.02.01

Three-Dimensional Coherent X-ray Surface Scattering Imaging in Grazing- Incidence Geometry. Jin Wang, Tao Sun, Zhang Jiang, Joseph Strzalka, Leonidas Ocola.

09:30-10:00am 09.02.02

Grazing Incidence Small Angle X-ray Scattering (GISAXS) Study of Nanoporous Polymer Thin Films. Hideaki Yokoyama.

10:00-10:30am Coffee Break

10:30-10:55am 09.02.03

Time-resolved Measurement on Dewetting Process of Polymer Blend Thin Films Using Specular and Off-specular Neutron Reflectometry Norifumi L. Yamada, Hiroki Ogawa, Rintaro Inoue, Toshiji Kanaya.

10:55-11:20am 09.02.04

Grazing Incidence Soft X-ray Scattering on Polymer Thin Films. Cheng Wang, Alexander Hexemer, Anthony Young, Howard Padmore.

11:20-11:35am 09.02.05

Combined GISAXS with Hard and Soft X-rays Applied to Phospholipid Alloy Films.

Hiroshi Okuda, Takayoshi Yamamoto, Kohki Takeshita, Mitsuhiro Hirai, Kitajima Kitajima, Hiroki Ogawa.

11:35-11:50am 09.02.06

Grazing-Transmission Scattering: A New Way to Measure Nanostructured Thin Films . Kevin Yager, Xinhui Lu, Danvers Johnston, Charles Black, Ben Ocko.

11:50-12:05pm 09.02.07

Stepwise Growth of DNA-nanoparticle Assembly on Substrate with Controlling Texture. Byeongdu Lee, Andrew J. Senesi, Daniel J. Eichelsdoerfer, Chad A. Mirkin.

13.05 Structure Validation

Edward Collins, Andrew Torelli, presiding

Lanai

09:00-09:30am 13.05.01

The Road to Scientific Serfdom. Bernhard Rupp.

09:30-10:00am 13.05.02

Model Building and Validation of Ligands using Coot. Paul Emsley.

10:00-10:30am Coffee Break

10:30-11:00am 13.05.03

Quality Assessment and Systematic Classification of Magnesium Binding Sites in RNA Crystal Structures. Ivan Shabalin, Heping Zheng, Katarzyna Mikolajczak, Wladek Minor.

11:00-11:30am 13.05.04

Validation of Crystallographic Models: from Diagnosis to Healing. Jane Richardson.

11:30-12:00pm 13.05.05

The New wwPDB Deposition and Annota-

Industrial SIG Meeting.....	12:00pm	Kohala/Kona
Canadian Division Meeting	12:00pm	Waianae
Joint SIG Meeting: Neutron/Materials/Powder	5:00pm	Oahu/Waialua
Synchrotron Radiation SIG Meeting	5:00pm.....	Kohala/Kona
Poster Session M.....	5:30pm-7:30pm	Ballroom
Bruker Mixer (invitation only).....		TBA

tion System. John Westbrook, Helen Berman, Gerard Kleywegt, John Markley, Haruki Nakamura, wwPDB Team.

13.06 Cool Structures

Richard Staples, presiding
Honolulu/Kahuku

09:00-09:15am **13.06.01**

Crystal Structure of the SBP-Tag:Streptavidin Complex Reveals a Novel Helical Scaffold for Developing Novel Biotechnology Reagents. Isabelle H Barrette-Ng, Sau-Ching Wu, Wai-Mui Tjia, Sui-Lam Wong, Kenneth Ng.

09:15-09:30am **13.06.02**

Asymmetric Binding of Metastasin (S100A4) to Non-muscle Myosin IIA. Gergely Katona, Annette Duelli, Bence Kiss, Laszlo Radnai, Katalin Kekesi, Ida Lundholm, Laszlo Nyitrai.

09:30-09:45am **13.06.03**

Structural Reorganizations Define the Interaction of Perforin with Calcium and the Lipid Membrane. Daouda Traore, Amelia Brenan, Ruby Law, Jamie Lopez, Kylie Brown, Gordon Llyod, James Whisstock, Iliia Voskiboinic.

09:45-10:00am **13.06.04**

Molecular Analysis of a G-actin Sensor. Stephane Mouilleron, Maria Wieszlak, Richard Treisman, Neil McDonald.

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

10:30-10:45am **13.06.05**

Crystal Structures of Tris(cyclooctyne) Complexes of Au, Ag, and Cu. Muhammed Yousufuddin, Chandrakanta Dash, Animesh Das, H. V. Rasika Dias.

10:45-11:00am **13.06.06**

Nanohoop Dreams: Crystal Structures of Cycloparaphenylenes, Derivatives and a Belted Buckyball. Jeffrey Bacon, Jianlong Xia, Matthew Golder, Elizabeth Hirst, Ramesh Jasti.

11:00-11:15am **13.06.07**

Anomalous X-Ray Diffraction and Complete Structural Refinement of Heterobimetallic Complexes of First-Row Transition Metals. Victor Young, Stephen Tereniak, Deanna Miller, Christopher Zall, Laura Clouston, Yu-Sheng Chen, Connie Lu.

11:15-11:30am **13.06.08**

Pushing the Limits: Giant Negative Linear Compressibility. Andrew Cairns, Jadna Catafesta, Claire Levelut, Jerome Rouquette, Arie van der Lee, Lars Peters, Amber Thompson, Vladimir Dmitriev, Matthew Tucker, Julien Haines.

11:30-11:45am **13.06.10**

Superspace Refinement of the (3+1)-Dimensional Incommensurately Modulated Phase of the Hydrated Sodium Salt of H-Acid a Commodity Dye Intermediate. Christopher Rackauckas, Jesse Rowsell.

13.07 Materials for a Sustainable Future

Olaf Borkiewicz, Peter Khalifah, presiding
Oahu/Waialua

09:00-09:20am **13.07.01**

Novel Tin Clathrates with the Cubic Type-II Structure. Svilen Bobev.

09:20-09:40am **13.07.02**

Crystal Structures and Properties of Bismuth Indium Oxide Sillenites. Michael Lufaso, Mary

MONDAY, JULY 22

Hertz, Daniel Arenas, Patricia Kalita, Kristina Lipinska, Diego Barbosa, William Paschoal.

09:40-10:00am **13.07.03**

Solar-Powered Molecular Machines: Materials Discovery of Single-Crystal Molecular Transducers via *in-situ* Photo-crystallography. Jacqueline Cole, Sven Sylvester.

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

10:30-10:50am **13.07.04**

Comprehensive Insights into the Structural and Chemical Changes in Next-generation Battery Electrodes During Cycling. Kamila Wiaderek, Olaf Borkiewicz, Karena M. Chapman, Peter J. Chupas.

10:50-11:10am **13.07.05**

Bifunctional $\text{La}_{1-x}\text{Ce}_x\text{Fe}_{1-y}\text{Mn}_y\text{O}_3$ Catalyst for Li-air Batteries with High Capacity and Cycle Life. Tiejun Meng, Mahbuba Ara, Lixin Wang, Simon Ng.

11:10-11:30am **13.07.06**

Enhanced Electrical Transport in Ordered Quantum Dot Nanocomposite Thin Films. Brandon Mercado, Aaron Kushner, Jason Tolentino, Bhavin Joshi, Zhibin Guan, Matt Law.

11:30-11:50am **13.07.07**

Hydrogen Storage Properties of the $2\text{LiBH}_4\text{-MgH}_2$ Reactive Hydride Composite Doped with Ti Additives and Al. Julian Puzkiel, Fabiana Gennari, Julio Andrade Gamboa, Pierre Arneodo Larochette.

13.08 Building Protein and Small Molecule Research Capacity at an Undergraduate Institution

Roger Rowlett, Kraig Wheeler, presiding Kohala/Kona

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

09:00-09:20am **13.08.01**

Protein Crystallography Research and Education at the University of Hawaii at Manoa. Ho Leung Ng.

09:20-09:40am **13.08.02**

Matching Crystallography with Student Needs and Ability. Bruce C. Noll, Michael Ruf, Joerg Kaercher.

09:40-10:00am **13.08.03**

Introducing Protein Crystallography to an Undergraduate Biochemistry Laboratory Course. Katherine Hoffmann.

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

10:30-10:50am **13.08.04**

The Value of Introducing X-ray Crystallography Across the Undergraduate Curriculum. Paul Baures.

10:50-11:10am **13.08.05**

Integrating Protein X-ray Crystallography into Undergraduate Teaching and Research at an Urban Comprehensive University. Emina Stojkovic.

11:10-11:30am **13.08.06**

Is Undergraduate Crystallographic Research the Scientific Equivalent of the "Art of the Possible"? William Ojala.

11:30-11:50am **13.08.07**

Integrating Chemical Crystallography into Advanced Undergraduate Laboratories: A Discovery Based Molecular Structure Determination Lab Module. Joseph Tanski.

11:50-12:00pm **13.08.08**

Mythbusters: 10 Things You May Have Heard

About Doing Protein Crystallography with Undergraduates That are not True and What to do About Them. Roger Rowlett.

01.01 Structural Enzymology (II) Nucleotide Metabolism Modification & Interactions

Hideki Aihara, Zachary Wood, presiding

Lanai

Funding for this session provided, in part, by Integrated DNA Technologies

01:30-02:00pm **01.01.01**
Crystal Structure of the Histone mRNA Stem-loop, Human Stem-loop Binding Protein and 3'hExo Ternary Complex. Dazhi Tan, William Marzluff, Zbigniew Dominski, Liang Tong.

02:00-02:30pm **01.01.02**
CRISPR Interference in Type I-C/Dvulg Organisms. Ailong Ke, Ki Hyun Nam.

02:30-03:00pm **01.01.03**
Structure and Function of Zucchini Endoribonuclease in piRNA Biogenesis. Osamu Nureki, Hiroshi Nishimasu, Hirotsugu Ishizu, Naoki Matsumoto, Haruhiko Siomi, Mikiko Siomi.

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

03:30-03:55pm **01.01.04**
The Ancient RIO Protein Kinases Function as ATPases in Ribosome Biogenesis. Nicole LaRonde, Vatsala Sagar, Irene Kiburu, Sebastien Ferreira-Cerca, Thorsten Schafer, Anne-Maria Wesseling, Momar Diop, Eileen Chai, Ed Hurt.

03:55-04:20pm **01.01.05**
Structural Insights into a Novel Mechanism of Toxicity and Neutralization of MqsR, a Ribonuclease Toxin. Dana Lord, Breann Brown, Wolfgang Peti, Rebecca Page.

04:20-04:45pm **01.01.06**
Crystal Structure of a RNA Polymerase II Transcribing Complex: Molecular Basis of DNA Tracking and Translocation. Guillermo Calero, Christopher Barnes, Monica Calero, Indranil Malik, Aina Cohen, Guowu Lin,

Ian Brown, Qiangmin Zhang, Filippo Pullara, Craig Kaplan.

04:45-05:10pm **01.01.07**
Crystal Structures of Human Norovirus Polymerase Complexes Trap the Enzyme in Different Parts of the Catalytic Cycle. Kenneth Ng, Dmitry Zamyatkin, Andrew Cottle, Dean Lang, Elesha Hoffarth, Gabriela Jurca, Hayeong Rho, Pawel Grochulski, Francisco Parra.

09.01 Dynamic & Flexible Structures in Biomolecules (II)

Yun-Xing Wang, presiding
Waianae

01:30-02:00pm **09.01.08**
Structural Insights into Cardiac Myosin Binding Protein C. Jill Trehwella.

02:00-02:30pm **09.01.09**
Picosecond Photobiology: Watching a Signaling Protein Function in Real Time via 100 Picosecond Time-Resolved X-ray Diffraction and Solution Scattering. Philip Anfinrud, Friedrich Schotte, Hyun Sun Cho, John Kyndt, Hironar Kamikubo, Mikio Kataoka.

02:30-03:00pm **09.01.10**
Comprehensive Objective Maps of Macromolecular Conformations by Quantitative SAXS Analysis. Greg Hura, Kevin Dyer, Cynthia McMurray, Helen Budworth, John Tainer.

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

03:30-03:45pm **09.01.11**
Effects of Nucleoid-associated Proteins on Bacterial Chromosome Structure. Michal Hammel, John Tainer, Dhar Amlanjyoti, Sankar Adhya.

03:45-04:00pm
Evolution of a New Fold- The Structure of Cyanuric Acid Hydrolase. Tom Peat, J. Newman, S. Balotra, M. Wilding, S. Panjkar, N. Cowieson, J. Holton, C. Scott.

MONDAY, JULY 22

04:00-04:15pm **09.01.12**
Structural Basis of the Regulation of Voltage-Gated Sodium Channels. Sandra Gabelli, Agedi Boto, Victoria Halperin Kuhns, Mario Bianchet, Federica Farinelli, Jean Jancocic, Gordon Tomaselli, L. Mario Amzel.

04:15-04:30pm **09.01.13**
Dissecting Thermodynamics of Large-scale Concerted Domain Motions Coupled with Ligand Binding During the Functional Cycle of Enzyme I. Jeong-Yong Suh.

04:30-04:45pm **09.01.14**
Conformational Constraints in Maltose Binding Protein Provide Insight into Chemical-Mechanical Coupling in ABC Transporters. Brian Shilton, Alister Gould.

04:45-05:00pm **09.01.15**
Structural Determinants of Pilin-Derived Protein Nanotube Oligomerization. Gerald Audette, Stephanie Lombardo, Anna Petrov, Darren Yong.

10.01 Interplay of Crystallography, NMR and Theoretical Methods
Ray Teller, presiding
Honolulu/Kahuku

01:30-02:00pm **10.01.01**
Organometallic Wheels Involving Ethylene and Coinage Metals. Rasika Dias, Mauro Fianchini, Charles F. Campana, Thomas R. Cundari, Vaclav Petricek.

02:00-02:30pm **10.01.02**
New Coordination Record for a Charged Buckybowl From X-ray Crystallography and ^7Li NMR. Marina Petrukhina.

02:30-03:00pm **10.01.03**
Electronic Communication in Mixed Early/Late Transition Metal Alkyne Complexes. Paul Raithby, Thomas Robinson, Andrew Johnson.

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

03:30-03:55pm **10.01.04**
IR, NMR, Electronic and Circular Dichroism Spectroscopy: Complementing X-ray and Neutron Diffraction Results. Larry R. Falvello, Milagros Tomas.

03:55-04:15pm **10.01.05**
Neutron Scattering Studies of Molecule Based Magnets. Javier Campo.

04:15-04:35pm **10.01.06**
Exotic Physics in Neutron Laue Diffraction. Garry McIntyre.

04:35-05:00pm **10.01.07**
Scientific Progress is Driven by Advances in Instrumentation: The Case of Neutron Scattering and Coordination Chemistry. Alberto Albinati.

11.03 Femtosecond X-ray Pulses: Biological Applications
Eaton Lattman, Dmitri Starodub, presiding
Kohala/Kona

01:30-02:00pm **11.03.01**
Femtosecond X-ray Crystallography. Uwe Weierstall.

02:00-02:30pm **11.03.02**
Continuous X-ray Nanocrystallography: The Approach for the Structural Analysis of "Real" Protein Nanocrystals. Ruben Dilanian, Victor Streltsov, Harry Quiney, Keith Nugent.

02:30-03:00pm **11.03.03**
A Comprehensive Method for Identifying and Prescreening Nanocrystals for Femtosecond Diffraction Experiments. Hilary Stevenson, Irimpan Mathews, Michael Soltis, Aina Cohen, Guillermo Calero.

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

03:30-04:00pm **11.03.04**
Employing the Reciprocal Space Autocorrelation Function for Structure Determination: From Nanoparticles to Biological Molecules.

Dmitri Starodub.

04:00-04:30pm **11.03.05**

Simultaneous fs X-ray Emission and X-ray Diffraction Measurement from Micro Crystals of Photosystem II. Jan Kern, Roberto Alonso-Mori, Rosalie Tran, Johan Hattne, Richard Gildea, Nthaniel Echols, Carina Gloeckner, Vittal Yachandra, Uwe Bergmann, Junko Yano.

04:30-05:00pm **11.03.06**

Fluctuation Scattering: SAXS at the Femtosecond Timescale. Peter Zwart, Billy Poon, Erik Malmerberg.

13.09 Materials for a Sustainable Future & Structure / Function of Metal-Organic Frameworks

Xiaoping Wang, presiding

Oahu/Waialua

01:30-02:00pm **13.09.01**

Tuning the Structure and Function of Metal-Organic Frameworks through Ligand Design. Hong-Cai Zhou.

02:00-02:20pm **13.09.02**

Unique Mechanism of Gas Sorption in a Selective Porous Network. Anna Plonka, Debasis Banerjee, William Woerner, Jing Li, John Parise.

02:20-02:40pm **13.09.03**

MOFs Under Pressure: The Reversible Compression of a Single Crystal. Kevin Gagnon, Christine Beavers, Abraham Clearfield.

02:40-03:30pm **Coffee Break**

03:30-03:50pm **13.09.05**

Stepwise Transformation of the Molecular Building Blocks in a Porphyrin- Encapsulating Metal-Organic Material. Zhenjie Zhang, Michael Zaworotko.

03:50-04:10pm **13.09.06**

Synthesis, Structural and Luminescence Studies of Uranyl Thiophene Carboxylate Coordination

Polymers: Effect of Ligand Sterics on Uranyl Coordination Modes. Sonia Thangavelu, Christopher Cahill.

04:10-04:30pm **13.09.07**

Structural Aspects of Organic Zeolite Behaviour. Janusz Lipkowski.

TUESDAY, JULY 23

Registration Desk.....	07:30am	Ballroom Foyer
Speaker Ready Room.....	07:30am	Iao Needle
Council Meeting Room.....	07:30am	Puna
Exhibit Show.....	10:00am	Ballroom

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

Cheryl Stevens, presiding

Lanai

08:00-08:45am

Eric Ortlund.

09.03 Membrane Protein Scattering

Shuo Qian, presiding
Waianae

09:00-09:30am

09.03.01

Detergent Organization Around Aquaporin-0 Revealed Using Small Angle X-Ray Scattering. Javier Perez, Alice Berthaud, John Manzi, Stephanie Mangenot, Alexandros Koutsioubas.

09:30-10:00am

09.03.02

From Soluble to Pore-forming: The Insertion of the Pro-apoptotic Protein Bax in Mitochondrial-like Lipid Membranes. Cecile Fradin, Dmitri Satsoura, Amit Patel, Kelly Cathcart, Sanjeevan Shivakumar, Brian Leber, David Andrews, Norbert Kucerka, John Katsaras.

10:00-10:55am Coffee Break

10:55-11:20am

09.03.04

Characterization of Lipid Matrices for Membrane Protein Crystallization by High-throughput Small Angle X-ray Scattering. Wei Liu, Jeremiah Joseph, Joshua Kunken, Thomas Weiss, Hiro Tsurutab, Vadim Cherezov.

11:20-11:45am

09.03.05

Understanding a Key Interaction in Exocytosis Using Small-Angle Neutron Scattering. Andrew Whitten, Michelle Christie, Gordon King, Ahu-Hong Hu, Russell Jarrott, Kai-En Chen, Anthony Duff, David James, Jenny Martin.

11:45-12:00

09.03.06

The Bio-SANS Effort on Membrane Protein Scattering. Shuo Qian, Sai Venkatesh Pingali, Volker Urban.

12.02 Etter Early Career Award Symposium

Albert Reger, presiding
Lanai

09:00-09:15am

12.02.01

PgaB is Required for the De-N-acetylation and Export of the Biofilm Polysaccharide PNAG. Dustin J Little, Grace Li, Joanna Poloczek, Ben DiFrancesco, Howard Robinson, Mark Nitz, Regis Pomes, P. Lynne Howell.

09:15-09:30am

12.02.02

HIV-1 Protease: Targeting Allosteric Sites to Overcome Drug Resistance. Theresa Tiefenbrunn, Stefano Forli, Ana Gonzalez, Michael Baksh, Max Chang, Yingssu Tsai, Ying-Chuan Lin, Alex Perryman, Jin-Khyu Rhee, Bruce Torbett, Arthur Olson, Mike Soltis, John Elder, M.G. Finn, C. David Stout.

09:30-09:45am

12.02.03

A Novel DNA Binding Mechanism for maf Basic Region-Leucine Zipper Factors Inferred from a MafA DNA Complex Structure and Binding Specificities. Xun Lu, Gerald Guanga, Cheng Wan, Robert Rose.

09:45-10:00am

12.02.04

Crystal Structures of a Condensation Domain Suggest Conformational Changes During the Synthetic Cycle of Nonribosomal Peptide Synthetases. Kristjan Bloudoff, Dmitry Rodionov, Thomas Martin Scheming.

10:00-10:30am

Coffee Break

TUESDAY, JULY 23

Agilent Luncheon	12:00pm.....	Royal Hawaiian Hotel -Regency Room III
Association's Annual Business Meeting	5:00pm.....	Kohala/Kona
Poster Session T	5:30pm-7:30pm.....	Ballroom

10:30-10:50am 12.02.05

Sub-Å Resolution X-ray Structure Details Aquaporin-water Interactions. Gerhard Fischer, Urszula Kosinska-Eriksson, Giray Enkavi, Rosmarie Friemann, Emad Tajkhorshid, Richard Neutze.

10:50-11:10am 12.02.06

Conformational Polymorphism. Aurora J Cruz-Cabeza, Joel Bernstein.

11:10-11:30am 12.02.07

Big Methods for Small Molecules. Karim Sutton, Richard Cooper, Kirsten Christensen, Amber Thompson, David Allan.

11:30-11:50am 12.02.08

Unit Cell Search Alternatives. Keith J McGill, Mojgan Asadi, Maria Toneva Karakasheva, Lawrence C. Andrews, Herbert J. Bernstein.

10:50-12:10pm 12.02.09

The Bond-Valence Model: Large-scale Evaluation of Bond-Valence Relations for Oxides. Olivier Gagne, Frank Hawthorne.

13.10 Reviewer Practices - Engaging New Crystallographic Reviewers

Peter Mueller, presiding
Kohala/Kona

09:00-09:20am 13.10.01

Should This Structure be Published? The Role of Reviewers. William Clegg.

09:20-09:40am 13.10.02

State-of-the-Art Crystallographic Refereeing. Ton Spek.

09:40-10:00am 13.10.03

Reviewing for Acta Cryst. C. Anthony Linden.

10:00-10:20am 13.10.04

Past, Present, and Future Ghosts in Submission, Review, and Archiving of Crystallographic Data in the American Chemical Society Journal Crystal Growth & Design. Robin Rogers.

10:20-10:40am Coffee Break

10:40-12:00pm Panel Discussion

13.11 Complementary Methods in Crystals and in Solution (I)

Michael Becker, Eric Ortlund, presiding
Oahu/Waialua

09:00-09:30am 13.11.01

High-Throughput Methods for Electron Crystallography. David Stokes, Nicolas Coudray, Ralph Lasala, Iban Ubarretxena-Belandia, Andreas Engel.

09:30-10:00am 13.11.02

Rotary ATPases in '4D'. Daniela Stock, Alastair Stewart, Lawrence Lee, Carol Robinson, Min Zhou.

10:00-10:30am Coffee Break

10:30-11:00am 13.11.03

Structure Activity Relationships of Nuclear Receptors, GPCRs and Kinases Revealed with Differential HDX. Patrick Griffin.

11:00-11:30am 13.11.04

High-Resolution Protein Structures by Magic-Angle Spinning NMR Spectroscopy. Chad Rienstra.

11:30-12:00pm 13.11.05

Structural and Dynamic Origins for the Ligand Binding Specificity Switch of a Tiam1 PDZ Domain Mutant. Xu Liu, David Speckhard, Tyson Shepherd, Ernesto Fuentes.

TUESDAY, JULY 23

TR.03 Transactions Symposium Neutron & Synchrotron Sources: Role in Crystallography (III): Emerging Characterization Facili- ties & Tools

Antonio dos Santos, Jonthan Hanson, presiding
Honolulu/Kahuku

09:00-09:30am

TR.03.01

Modulated-Enhanced Diffraction: Theory and Applications. Rocco Caliandro, Dmitry Chernyshov, Herman Emerich, Marco Milanese, Luca Palin, Atsushi Urakawa, Wouter van Beek, Davide Viterbo.

09:30-10:00am

TR.03.02

Quantitative Neutron Diffraction at Megabar Pressures. Malcolm Guthrie, Reinhard Boehler, Christopher Tulk, Jamie Molaison, Antonio dos Santos, Kuo Li, Russell Hemley.

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

10:30-11:00am

TR.03.03

Single-particle Diffraction Imaging using X-ray Free-electron Lasers. Stefan Hau-Riege.

11:00-11:20am

TR.03.04

Time-Resolved Measurements of Lattice Distortion in Ferroelectric Crystals Induced by Application of Electric Field: Single Crystal Diffraction Study. Chikako Moriyoshi.

11:20-11:40am

TR.03.05

Recent Progress Towards 3D Tomographic Imaging of Strains using Neutrons. Brian Abbey, Shu-Yan Zhang, Henry Kirkwood, Alexander Korsunsky.

11:40-12:10pm

TR.03.06

Emerging Capabilities for Materials Characterization with Polychromatic Microdiffraction. Gene Ice, Bennett Larson, Jonathan Tischler, John Budai, Eliot Specht, Judy Pang.

13.11 Complementary Methods in Crystals and in Solution (II)

Brian Shilton, Eddie Snell, presiding
Oahu/Waialua

01:30-02:00pm

13.11.06

Protein Nanocrystal Detection by Nonlinear Optical Imaging. Garth Simpson.

02:00-02:30pm

13.11.07

Polarization-resolved Second Harmonic Generation Microscopy for Identification of Multidomain Protein Crystals. Emma DeWalt, Victoria Begue, Judith Ronau, Shane Sullivan, Chittaranjan Das, Garth Simpson.

02:30-03:00pm

13.11.08

Structure, Dynamics, Evolution and Function of a Major Scaffold Component in the Nuclear Pore Complex. Seung Joong Kim, Parthasarathy Sampathkumar, Paula Upla, William Rice, Jeremy Phillips, Benjamin Timney, Javier Fernandez-Martinez, Andrej Sali, Michael Rout, Steven Almo.

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

03:30-04:00pm

13.11.09

Using Single Crystal Spectroscopy to Your Advantage: The Case of the Missing Ferryl Iron. Carrie Wilmot, Erik Yukl, Riti Sarangi, Lyndal Jensen.

04:00-04:30pm

13.11.10

Bridging Solutions and Crystals by Electron Paramagnetic Resonance Spectroscopy of Dynamic Macromolecules. Betty J. Gaffney.

04:30-05:00pm

13.11.11

Beyond the Kinase Domain: Challenges in Designing Allosteric Inhibitors. Nicole Caspers, Ann Aulabaugh, Seungil Han, Francis Rajamohan, Weigong Ding, Hong Wang, Robert Czerwinski, Lise Hoth, Jeffrey Ohren, Quintus Medley, Christoph Zapf, David Limburg, David Anderson, Ravi Kurumbali.

13.12 Structural Genomics for the Home Lab - Membrane Proteins**George Lountos, Ward Smith, presiding**
Lanai**01:30-02:00pm** **13.12.01**
High Throughput Microscale Membrane Protein Thermostability Assays. Thomas Tomasiak, Bjorn Pedersen, Sarika Chaudhary, Shujun Yuan, Andrew Rodriguez, Yaneth Robles, Robert Stroud.**02:00-02:30pm** **13.12.02**
GPCR with New Fusion Partners Yield High-Resolution Insights and Novel Structures. Wei Liu, Eugene Chun, Aaron Thompson, Chong Wang, Huixian Wu, Vsevolod Katritch, Gye Won Han, Vadim Cherezov, Raymond Stevens.**02:30-03:00pm** **13.12.03**
Robust Tools for Successful Membrane Protein Data Collection. Nagarajan Venugopalan, Ruslan Sanishvili, Mark Hilgart, Sudhir Babu Pothineni, Craig Ogata, Sergey Stepanov, Michael Becker, Oleg Makarov, Janet Smith, Robert Fischetti.**03:00-03:30pm** **Coffee Break****03:30-03:50pm** **13.12.04**
PSI Structural Biology Knowledgebase: New Ways to Enable Membrane Protein Research. Margaret Gabanyi, Paul Adams, David Micallef, Wladek Minor, William McLaughlin, Torsten Schwede, Raship Shah, Yi-Ping Tao, John Westbrook, Helen Berman.**03:50-04:10pm** **13.12.05**
The PSI:Biological-Materials Repository: A Resource for Protein Expression Plasmids. Catherine Seiler, Jin Park, Michael Fiacco, Jason Steel, Preston Hunter, Andrea Radtke, Amit Sharma, Casey Sedillo, Joshua LaBaer.**04:10-04:30pm** **13.12.06**
Identification of Optimal Membrane Protein Candidates for X-Ray Crystallography. Nilou Ataie, Jared Kim, Allison Kagawa, Il Cho, Qingxiao Li, Ho Leung Ng.**04:30-04:50pm** **13.12.07**
Crystal Structure of the Transhydrogenase Membrane Component in the Lipidic Cubic Phase. Josephine Leung, Mutsuo Yamaguchi, Lici Ariane Schurig-Briccio, Wei Liu, Arne Moeller, Bridget Carragher, Clinton S. Potter, Robert B. Gennis, Vadim Cherezov, C. David Stout.**13.14 Materials Discovery****Daniel Shoemaker, Fernando Uribe-Romo, presiding**
Kohala/Kona**01:30-01:50pm** **13.14.01**
Predicting New Materials via Evolutionary Algorithms. Qiang Zhu, Artem Oganov.**01:50-02:10pm** **13.14.02**
The Materials Project: A Computational Approach to Community-Driven Materials Discovery. Anubhav Jain, Shyue Ping Ong, Geoffroy Hautier, Shreyas Cholia, Daniel Gunter, Wei Chen, William Richardson, David Skinner, Gerbrand Ceder, Kristin Persson.**02:10-02:40pm** **13.14.03**
Algorithms for Crystal Structure Solution of Complex Zeolites using Powder Diffraction Data. Christian Baerlocher, Lynne McCusker.**02:40-03:00pm** **13.14.04**
A Zeolitic 'Chatterbox': Pressure-Induced Hydration and Structural Inversions in Natrolites. Yongjae Lee, Donghoon Seoung, Thomas Vogt, Chi-Chang Kao.**03:00-03:30pm** **Coffee Break****03:30-04:00pm** **13.14.05**
In-situ Investigations of Chemical Reactions using X-ray Scattering Techniques. Wolfgang Bensch.**04:00-04:20pm** **13.14.06**
Designing Fluoride and Oxyfluoride Materials for Low or Negative Thermal Expansion by Manipulating Composition, Disorder and Dimensionality. Angus Wilkinson, Cody

TUESDAY JULY 23

Morelock, Justin Hancock, David Kakalios, Christopher Monaco.

04:20-04:40pm **13.14.07**

Sterically Directed Chalcogenides: Self-Assembling Superstructures of n-Dimensional Materials. J. Nathan Hohman, Hao Yan, Arturas Vailionis, Nicholas Melosh.

04:40-05:00pm **13.14.08**

Sulfate Assisted Assembly of Zirconium Hydroxo/oxo Sulfate Clusters. Karah Knope, Yung-Jin Hu, S. Skanthakumar, Travis Bray, L. Soderholm.

13.15 Contemporary Crystal Engineering (I)

Len Barbour, Travis Holman, presiding
Waianae

01:30-02:00pm **13.15.01**

Porosity in Flexible Metal-organic Systems. Len Barbour.

02:00-02:30pm **13.15.02**

Towards Improved Frameworks for Gas Separations: Establishing an Atomistic Picture of Gas Sorption Through Complimentary Experimental Techniques. Paul Forster, Keith Lawler, Zeric Hulver.

02:30-03:00pm **13.15.03**

Separation of Xenon and Krypton using Metal Organic Frameworks. Praveen Thallapally, Jian Liu, Denis Strachan.

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

03:30-03:50pm **13.15.04**

Gas-solid Reactions in Non-porous Crystalline Materials Studied by *in situ* XRPD. Inigo Vitorica Yrezbal, Guillermo Minguez-Espallargas, Adrian Hill, Lee Brammer.

03:50-04:10pm **13.15.05**

Dynamic Crystal to Crystal Transformations via Coordination Polymers. Robert Burrow, Giancarlo Belmonte, Catilene Dalla Barba.

04:10-04:30pm **13.15.06**

Molecular Disorder as a Tool in the Crystal Engineering Toolkit. Lynne Thomas, Charlotte Jones, Chick Wilson.

04:30-05:00pm **13.15.07**

Co-Crystal Design using the Cambridge Structural Database. Peter Wood, Neil Feeder, Matthew Furlow, Peter Galek, Elna Pidcock.

05:00-05:30pm **13.15.08**

The Interplay Between Intermolecular Forces in Cocrystals of Pyrazinamide. Heba Abourahma, Jesus Melendez, Breanne Cullen, Rachita Rai.

TR.04 Transactions Symposium Neutron & Synchrotron Sources: Role in Crystallography (IV): Chemical Crystallography

Christine Beavers, Simon Teat, presiding
Honolulu/Kahuku

01:30-02:00pm **TR.04.01**

Synchrotron Single-crystal Diffraction for Chemists: Development and Maturity. William Clegg.

02:00-02:30pm **TR.04.02**

Non-ambient Synchrotron Diffraction Studies in Molecular Materials Chemistry. Paul Raithby, Mathew Bryant, Lauren Hatcher, Christopher Woodall.

02:30-03:00pm **TR.04.03**

Crystallographic Transitions Coupled to Spin Crossover in Molecular Complexes Uncovered by Synchrotron X-ray Diffraction. Guillem Aromi, Jose Sancez Costa, Gavin Craig, Simon Teat, Christine Beavers, Olivier Roubeau.

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

03:30-04:00pm **TR.04.04**

Studies of Molecular Structural Evolution Enabled by Advanced Sources. Chick Wilson.

04:00-04:30pm

TR.04.05

Structural Studies of Gas Adsorbed Metal-Organic Frameworks. Wendy L. Queen, Craig M. Brown, Eric D. Bloch, Jeffrey R. Long, Matthew R. Hudson.

04:30-05:00pm

TR.04.06

Structure of Surprising Non-isolated Pentagon Rule Endohedral Metal Carbide made Possible by Synchrotron Radiation. Marilyn Olmstead, Alan Balch, Faye Bowles, Luis Echegoyen, Jianyuan Zhang, Harry Dorn, Christine Beavers.

13.21 Enabling Partnerships for Broader Crystallographic Data Accessibility

Joe Reibenspies, Thomas Terwilliger, John Westbrook, presiding
Honolulu/Kahuku

Funding for this session provided, in part, by Agilent Technologies, Bruker AXS, Cambridge Crystallographic Data Centre

07:30-07:45pm

13.21.01

The Powder Diffraction File: Produced and Delivered through Worldwide Partnerships. Timothy Fawcett, Cyrus Crowder, Soorya Kabekkodu.

07:45-08:00pm

13.21.02

The Cambridge Structural Database: A Future of Compromise or Ideality Open to the Future. Colin Groom, Ian Bruno.

08:00-08:15pm

13.21.03

The wwPDB: Ensuring a Single, Uniform Archive of High Quality Data. Helen Berman, Gerard Kleywegt, John Markley, Haruki Nakamura.

08:15-08:30pm

13.21.04

The Crystallography Open Database in its 11th Year. Peter Moeck, Daniel Chateigner, Robert T. Downs, Saulius Grazulis, Armel Le Bail, Luca Lutterotti, Miguel Quiros.

ACA Members' Business Meeting

5:00pm

Kohala/Kona

All are welcome

WEDNESDAY, JULY 24

Registration Desk.....	07:30am	Ballroom Foyer
Speaker Ready Room.....	07:30am	Iao Needle
Council Meeting Room.....	07:30am	Puna
Awards Banquet (ticket required).....	6:30pm	Royal Hawaiian Hotel, Monarch Room

AW.04 Trueblood Award Presentation and Lecture

Cheryl Stevens, presiding

Lanai

08:00-08:45am AW.04.01

Automated Structure Solution, Density Modification, And Model Building For MAD, SAD AND MIR. Thomas Terwilliger.

01.02 Host Pathogen Interactions

Graeme Conn, Erica Saphire, presiding

Lanai

Funding for this session provided, in part, by Appropriate Technical Resources, Inc., Bruker AXS, Molecular Dimensions, Virology Journal-Biomed Central, Wyatt Technology

09:00-09:15am

01.02.01

Structural Basis for Haemoglobin Capture by *S. aureus*- Stealing Haem from Haemoglobin. Kaavya Krishna Kumar, David Jacques, Tom Caradoc-Davies, Thomas Spirig, Reza Mallirchegini, Claire Dickson, Joel Mackay, Robert Clubb, J. Mitchell Guss, David Gell.

09:15-09:30am

01.02.02

Structure of a Mycobacteriophage Xis Reveals a Domain-swapped Filament that Promotes DNA Bending and Constrains Intasome Architecture During Excision. Andrew VanDemark, Shweta Singh, Joseph Plaks, Nickolas Homa, Christopher Amrich, Annie Heroux, Graham Hatfull.

09:30-10:00am

01.02.03

Genotype-dependent Glycan Specificity in Rotaviruses - Evolution of a New Paradigm. Bidadi Prasad, Liya Hu, Nicolas Cortes-Penfield, Sasirekha Ramani, Sue Crawford, Rita Czako, Gagandeep Kang, Jacques Le Pendu, David Smith, Mary Estes.

10:00-10:30am Coffee Break

10:30-10:50am

01.02.04

Ebola Virus VP40 Makes Multiple Structures for Multiple Functions. Erica Ollmann Saphire, Zachary Bornholdt, Takeshi Noda, Dafna Abelson, Peter Halfmann, Malcolm Wood, Yoshihiro Kawaoka.

10:50-11:10am

01.02.05

Structure of Human Cytomegalovirus UL141 in Complex with TRAIL-R2 Reveals Different Receptor Engagement Compared to Endogenous Ligand TRAIL. Dirk Zajonc, Ivana Nemcovicova, Chris Benedict.

11:10-11:25am

01.02.06

Structural Basis for the Recognition of 5'-Triphosphate Viral RNA by Human IFIT Proteins. Yazan Abbas, Andreas Pichlmair, Maria W. Gorna, Giulio Superti-Furga, Bhushan Nagar.

11:25-11:45am

01.02.07

Rational HIV Immunogen Design to Target Specific Germline B Cell Receptors. Jean-Philippe Julien, Joseph Jardine, Sergey Menis, Takayuki Ota, Oleksandr Kalyuzhnyi, Dennis Burton, Andrew Ward, David Nemazee, William Schief, Ian Wilson.

11:45-12:00pm

01.02.08

Targeting the g-Herpesvirus Bcl-2-Mediated Inhibition of Autophagy and Apoptosis. Sangita Sinha, Minfei Su, Yang Mei, Christopher Colbert.

03.02 General Interest (II)

Allen Oliver, Jeanette Krause, presiding

Honolulu/Kahuku

09:00-09:20am

03.02.01

Facilitation of Nucleic Acid Crystallization and Phasing by Selenium-Nucleic Acids. Zhen Huang, Wen Zhang, Sibao Zhang, Huiyan Sun, Julianne Caton-Williams.

WEDNESDAY, JULY 24

09:20-09:40am

A Lesson in Phase Transitions. Carla Sleboznick, David Hobart, Joseph Merola.

03.02.02

09:30-10:00am

The Quest for Ultra-high Resolution: Lessons from 19-ID at the APS. Julian Chen, Stephan Ginell, Gerd Rosenbaum, Andrzej Joachimiak.

11.04.02

09:40-10:00am

Comparing Single Crystal and Powder XRD Instruments for Routine Quantitative Powder Analyses. Stacey Smith, Peter Mueller.

03.02.03

10:00-10:30am Coffee Break

10:00-10:30am Coffee Break

10:30-10:50am

Crystallization and Diffraction: A One Hour Experiential Learning Core Science Standard Lesson for Grade 5. Colleen Lopez, Jon Rocha, Eric Reinheimer, Bianca Mothe, Bernhard Rupp, Katherine Kantardjieff.

03.02.04

10:30-10:50am

Optimizing the Set-Up of a Regular Macromolecular Crystallography Beamline for Ultra-High Resolution Crystallography. Gerd Rosenbaum, Stephan Ginell, Julian Chen.

11.04.03

10:50-11:20am

PILATUS 12M-DLS - A Specific Detector Solution for Long-wavelength Phasing Experiments. Clemens Schulze-Briese.

11.04.04

10:50-11:10am

Precipitant Chirality and Protein Crystallization. Neer Asherie, Mark Stauber, Jean Jakoncic, Jacob Berger, Jerome Karp, Ariel Axelbaum, Dahniel Sastow, Sergey Buldyrev, Bruce Hrnjez.

03.02.05

11:20-11:40am

Macromolecular Crystallography at Higher Energy. Jean Jakoncic, V. Stojanoff, V. Honkimaki.

11.04.05

11:10-11:30am

Trace Fluorescent Labeling for Protein Crystallization Screening. Marc Pusey, Michelle Morris, Qunying Yuan, Jorge Barcena, Joseph Ng.

03.02.06

11:40-12:00pm

The MDS (Multiple-Dataset) Approach and its Implications for Dose Reduction. John Rose, Unmesh Chinte, Zheng-Qing (Albert) Fu, Hua Zhang, Lirong Chen, John Chrzas, Bi-Cheng Wang.

11.04.06

11:30-11:50am

Looking for Light Atoms in Lithium-ion Battery Materials. Peter Khalifah.

03.02.07

13.15 Contemporary Crystal Engineering (II)

**Heba Abourahama, Tomislav Friscic, presiding
Waianae**

11.04 Specialized MX Experiments

**Stephan Ginell, Gerd Rosenbaum, presiding
Kohala/Kona**

09:00-09:30am

X-ray and Optical Wave Mixing. Ernest Glover, Jerome Hastings, David Fritz, Marco Cammarata, David Reis, Steven Harris, Thomas Allison, Jan Feldkamp.

11.04.01

09:00-09:30am

In situ Combined Multi-technique Approach to Material Synthesis: What Can Be Learned from *in situ* X-ray Scattering and Absorption Methods. Eli Stavitski.

13.15.09

09:30-10:00am

Structure-properties Relations of Adsorption in Porous Materials. Matthew Hudson, Craig Brown, Wendy Queen, Jarad Mason, Eric Bloch, Jeffery Long, Raul Lobo.

13.15.10

10:00-10:30am Coffee Break

WEDNESDAY, JULY 24

10:30-11:00am **13.15.11**
Unlocking New Materials with the Use of Elevated Pressures. Saul Lapidus, Greg Halder, Karena Chapman, Peter Chupas, John Schlueter.

11:00-11:20am **13.15.12**
Engineering Crystalline Cavities for Highly Selective Gas Enclathration and Confinement. K. Travis Holman, Christopher Kane.

11:20-11:40am **13.15.13**
Solid-state Synthesis and Isolation of Reactive Intermediates using Mechanochemistry: The Synthesis of Aromatic N-thiocarbamoylbenzotriazoles. Vjekoslav Strukil, Tomislav Friscic.

11:40-12:00pm **13.15.14**
Solid-state Reactivity by Milling and Aging as the Basis for a System of Cleaner and More Efficient Synthesis of Molecules and Materials. Tomislav Friscic.

13.17 Microstructural Evolution (Mesoscale)/Geologic Catalytic and Engineering

Ken Littrell, presiding
Oahu/Waialua

09:00-09:30am **13.17.01**
Solvent Effects on Pore Size and Structure of Natural Organic Matter. Lee Hoffman, Ken Littrell, James Rice.

09:30-10:00am **13.17.02**
Small-angle Neutron Scattering Study of the Oxidation of Alumina- and Chromia-forming Stainless Steels. Ken Littrell, G. Rother, J.R. Keiser, K.A. Uncoic, L.M. Anovitz, R.A. Peascoe-Meisner, M.L. Santella, D.J. Wesolowski, D.R. Cole.

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

10:30-11:00am **13.17.03**
Small Angle Neutron Scattering and Imaging Analysis of Multiscale Porosity in the St. Peter Sandstone: Analytical and Experimental Results. Lawrence Anovitz, David Cole, Gernot

Rother, Ken Littrell, Lawrence Allard.

11:00-11:30am **13.17.04**
Small Angle Neutron Scattering Applied to Nuclear Materials. Nicholas Cunningham, Yuan Wu, Peter Wells, G. Robert Odette.

11:30-12:00pm **13.17.05**
SANS Study of Highly Irradiated RPV Steels. Mikhail Sokolov, Randy Nanstad, Ken Littrell.

03.02 General Interest (III)

Jeanette Krause, Allen Oliver, presiding
Honolulu/Kahuku

01:30-01:50pm **03.02.08**
HyP - Hydrogen Atom Positions from Electron Density Maps. Ho Leung Ng, Matthew Bronstad.

01:50-02:10pm **03.02.09**
ProMOL 5. Maria Karakasheva, Madolyn MacDonald, Mikhail Osipovitch, Cyprian W. Corwin, Paul A. Craig, Herbert J. Bernstein.

02:10-02:30pm **03.02.10**
NuProPlot: Nucleic Acid and Protein Interaction Analysis and Plotting Program. Lagnajeet Pradhan, Hyun-Joo Nam.

02:30-02:50pm **03.02.11**
Accelerating Structure Refinement by Predicting Side Chain Conformations Using Real Space Data. Przemyslaw Porebski, Marcin Cymborowski, Wladek Minor.

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

03:30-03:50pm **03.02.12**
Structure and Receptor Complexes of the Hemagglutinin from a Highly Pathogenic H7N7 Influenza Virus. Hua Yang, Paul Carney, Ruben Donis, James Stevens.

03:50-04:10pm **03.02.13**
Structure Determination of SLAP2 from a Double Lattice Crystal Reveals Close Association of its SH3 and SH2 Domains. Leanne

Wybenga-Groot, C. Jane McGlade.

04:10-04:30pm **03.02.14**

Rotational Order-disorder Structures of Fluorescent Proteins FP480 and rsTagRFP. Sergei Pletnev, Fedor Subach, Vladislav Verkhusha, Zbigniew Dauter.

04:30-04:50pm **03.02.15**

Acoustic Droplet Ejection for Nanoliter Scale Crystallization Trials. Ping Wu, Seth Harris.

04.01 From Knowledge to Design: Data Mining in Materials Chemistry

Susan Reutzler-Edens, Peter Wood, presiding
Oahu/Waialua

01:30-02:00pm **04.01.01**

A Chemical View of How and When What Crystallized with Whatever in the ~ 625,000 Crystal Structures of the Cambridge Structural Database (as534be = 2012 release). Jack Gougoutas, Michael Galella.

02:00-02:30pm **04.01.02**

Correlation of Disorder with Crystal Growth Conditions using Structure Solution from Powder Diffraction Data, Single Crystal Structure Determination, Solid State NMR and Computational Modeling. Matthew Peterson, Yuan-Hon Kiang, Karthik Nagapudi, Tian Wu.

02:30-03:00pm **04.01.03**

A Common Supramolecular Motif in the Alkali Metal Salts of "H-Acid", Including the Incommensurately Modulated Phase of the Commercially Important Sodium Hydrate. Jesse Rowsell, Christopher Rackauckas, James Rosenberger.

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

03:30-04:00pm **04.01.04**

Similar But Different - A Case of Crystal Form Diversity, Salt Similarity and Structure/property Relationships. Magali Hickey, Tarek Zeidan, Mark Oliveira, Peter Wood, Orn Almarsson.

04:00-04:30pm **04.01.05**

Probing Crystal Structures by Single-Point Molecular Perturbation in a Family of 11-Azaartemisinin Derivatives. Ian D Williams, Cathy Cheu, Herman H-Y Sung.

04:30-05:00pm **04.01.06**

Reducing Structure-Space Dimensionality *via* Machine Learning. Wenhao Sun, Stephen Dacek, Gerbrand Ceder.

13.18 Nanodomains & Beyond

Craig Bridges, Antonio dos Santos, presiding
Waianae

01:30-02:00pm **13.18.01**

Nanodomains in Functional Materials. John Claridge.

02:00-02:30pm **13.18.02**

The Prediction and Experimental Observation of Compositional Order in Binary Platinum Alloys. Branton J. Campbell, Chumani Mshumi, Candace I. Lang, Lauren R. Richey, K.C. Erb, Richard R. Vanfleet, Gus L. W. Hart.

02:30-02:50pm **13.18.03**

A Neutron Diffraction Investigation of the Solid-Solution $\text{Na}_2(\text{Zn},\text{Co})\text{SiO}_4$. Rebecca Beadling, Ashfia Huq, Charles Lake.

02:50-03:30pm **Coffee Break**

03:30-04:00pm **13.18.04**

Quantifying Stacking Disorder in Topochemically-Converted Layered Oxides Using Real-Space Models. Scott Misture, Eric Nichols.

04:00-04:30pm **13.18.05**

Gamma Profile Analysis for Stress, Texture, Grain Size and Crystal Orientation. Bob He.

04:30-05:00pm **13.18.06**

Some Garnets are Cubic and Birefringent, Why? Styte Antao, Allison Klincker, Stephanie Round.

WEDNESDAY, JULY 24

13.20 Exciting Structures

Angeline Lyon, presiding

Lanai

Funding for this session provided, in part, by Rayonix

01:30-02:00pm **13.20.01**

Structural Insights into Muscarinic Acetylcholine Receptor Function. Andrew Kruse.

02:00-02:30pm **13.20.02**

Symmetry Enhancement in a Layered Hexagonal Protein Structure. Michael Thompson, Todd Yeates.

02:30-03:00pm **13.20.03**

Cholesterol Hepatic Internalization Decoded by X-rays. Hay Dvir, Mehul Shah, Enrico Girardi, Marilyn Farquhar, Dirk Zajonc.

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

03:30-04:00pm **13.20.04**

Allosteric Inhibition of a Class Ia Ribonucleotide Reductase is Mediated by Structural Interconversions. Christina Zimanyi, Nozomi Ando, Edward Brignole, Michael Funk, Francisco Asturias, JoAnne Stubbe, Catherine Drennan.

04:00-04:30pm **13.20.05**

Insights into the Catalytic Region of Human Transmembrane Glycoprotein UCE from the Crystal Structure of a Novel Bacterial Homolog. Debanu Das, Wang-Sik Lee, Ashley Deacon, Stuart Kornfeld, Ian Wilson.

04:30-05:00pm **13.20.06**

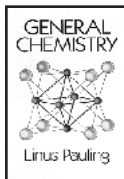
Exploring the Mechanism of Spliceosome Assembly: Structural, Genetic and Biophysical Analyses of the U6 snRNA/Prp24 Binary Complex. Eric Montemayor, Allison Didychuk, Ashley Richie, Elizabeth Curran, Christine Treba, Samuel Butcher, David Brow.

THURSDAY, JULY 25

**2014 Meeting
Planning Session**

09:00-11:00am Kohala/Kona

POSTER PRIZES



Pauling Poster Prize, Canadian and IUCr Poster Prize

The Pauling Poster Prize established by the ACA and is supported by member contributions, to honor Linus Pauling. Pauling was one of the pioneers in American structural research and was very supportive of the ACA. At each annual meeting, the five best graduate or undergraduate poster presentations receive Pauling awards. Each award consists of \$200, a complimentary banquet ticket, and a copy of a Linus Pauling book.

An additional Pauling Prize sponsored by the Canadian Division

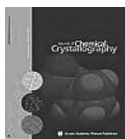


of the ACA and the Canadian National Committee of the IUCr, will be given to the highest ranked graduate or undergraduate poster from a Canadian laboratory. Honorable mention awards for this prize are also made; they consist of a complimentary banquet ticket.



IUCr Poster Prize

The IUCr Executive Committee is pleased to continue a series of IUCr awards presented at meetings of the regional affiliates and national crystallographic associations. The award is complimentary online access to all IUCr journals for one year or a complimentary volume of International Tables or other IUCr publication.



Journal of Chemical Crystallography Prize

The best graduate or undergraduate 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 graduate or undergraduate 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 meeting.



Oxford Cryosystems Low Temperature Poster Prize

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



Taylor & Francis Biomolecular Crystallography Poster Prize

This prize is open to all participants and is awarded to the best poster describing a successful application of a non-routine or computationally challenging structure solution and refinement technique in biomolecular crystallography. The winner will receive Bernhard Rupp's book Biomolecular Crystallography donated by the Taylor & Francis Group and will be announced at the banquet on Wednesday.

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

Crystallization of Proteins in Electric Fields. Evgeniya Rubin, Vivian Stojanoff.

S-02

α -glucosidase-1, a Key Enzyme in Eukaryotic N-glycosylation: Crystal Structure and Basis for Substrate Specificity. David Rose, Megan Barker.

S-03

Temperature Dependence of Thermolysin Kinetic and Structural Phase Transitions. Ming Dong, Brian Bahnsen.

S-04

Catalytic Assembly of Eukaryotic RNase III: How Rnt1p Recognizes the Conserved AGNN Tetraloop and Measures Down. Xinhua Ji, Yu-He Liang, Mathieu Lavoie, Marc-Andre Comeau, Sherif Abou Elela.

S-05

The Cerebral Cavemous Malformation-2 (CCM2) Protein Contains a C-terminal Domain. Oriana Fisher, Rong Zhang, Xiaofeng Li, James Murphy, Borries Demeler, Titus Boggan.

S-06

Crystal Structure of KLHL3 in Complex with Cullin3. Alan Ji, Gilbert Prive.

S-07

Trapping Intramolecular (cis) and Intermolecular (trans) Acyl-enzyme Complexes in Viral

Proteases that Utilizes a Ser-Lys Dyad Mechanism. Mark Paetzel, Ivy Yeuk Wah Chung.

S-08

Serial Femtosecond Crystallography with Micrograms. Raymond Sierra, Hartawan Laksmo, Michael Bogan.

S-09

Exploiting the Structure and Mechanism of Viral Deubiquitinases to Engineer Improved Live-virus Vaccines. Brian Mark, Puck van Kasteren, Ben Bailey-Elkin, Terrence James, Dennis Ninaber, Corrine Beugeling, Mazdak Khajehpour, Eric Snijder, Marjolein Kikkert.

S-10

Structural Insights of Outer Membrane Protein Methyltransferases from Rickettsia. Amila Abeykoon, Nicholas Noinaj, Chien-Chung Chao, Guanghui Wang, P. Boon Chock, Marjan Gucek, Wei-Mei Ching, Susan K. Buchanan, David C. H. Yang.

S-11

Sulfoxide-Bound Crystal Structure of a Baeyer-Villiger Monooxygenase. Michelle McEvoy, Brahm J. Yachnin, Peter C. K. Lau, Albert M. Berghuis.

S-12

X-ray Phase Measurements as a Probe of Small Structural Changes in Engineered Materials of Technological Relevance. Zohrab Amirkhanyan, Claudio M.R. Remedios, Sergio L. Morelhaio.

Posters-S

S-13

Structural Basis for the Inhibition of *Mycobacterium tuberculosis* L,D-Transpeptidase by Meropenem. HyounSook Kim, Byung Woo Han, Se Won Suh.

S-14

Structural and Functional Characterization of HP0377, a Thioredoxin-fold Protein from *Helicobacter pylori*. Ji Young Yoon, Se Won Suh.

S-15

Computation and Utilization of Synthetic Diffraction Data for Structural Characterization of Nanomaterials. Hande Ozturk, Hanfei Yan, John P. Hill, I. Cevdet Noyan.

S-16

X-Ray Structural Analysis of Chiral Aspects of Antiepileptic Drugs Containing an α -Substituted Amide Group. Bhupinder Sandhu, Samuel Bentum, Alexandr Fonari, Victor N. Khrustalev, Arcadius V. Krivoshein, Tatiana Timofeeva.

S-17

Fully Indium-Exchanged Zeolite Y Reacts with Oxygen to Form cyclo-Ozone Rings and Framework Peroxides. Cheol Woong Kim, Jong Jin Kim, Hyeon Seung Lim, Joon Young Kim, Nam Ho Heo, Karl Seff.

S-18

Structural and Functional Analysis of Splicing Factor Prp28. Lingdi Zhang, Tao Xu, Rui Zhao.

S-19

X-ray Induced Photo-reduction of Cu(II) Mediated by Glycerol as a Glassing Agent. Kurt Nienaber, M. Jake Pushie, Ingrid Pickering, Graham George.

S-20

n-type Ferrocene Dopants for Organic Thin-Film Transistors. Evgheni Jucov, Siyuan Zhang, Benjamin Naab, Zhenan Bao, Stephen Barlow, Seth Marder, Tatiana Timofeeva.

S-21

Evidence for R-State Stabilization of *Haemophilus influenzae* β -Carbonic Anhydrase by the N-terminal α -Helix. Regan Esposito, Thomas Mancuso, Krutika Ravi, Hilary Nicholson, Claire Maggioletto, Sam Wopperer, Roger Rowlett.

S-22

Investigation of Intersubunit Communication in *Haemophilus influenzae* β -Carbonic Anhydrase Using N-Terminal Helix Point Variants. Thomas Mancuso, Amanda Harris, Michelle Lu, Krutika Ravi, Roger Rowlett.

S-23

Crystal Structures of S-HPCDH Reveal Determinants of Stereospecificity for R- and S-hydroxypropyl-coenzyme M Dehydrogenases. Jeremy Bakelar, Dariusz Sliwa, Johnson Sean.

S-24

Insight into Tubulin Poly-glutamylolation by TLL7. Christopher Garnham, Antonina Roll-Mecak.

S-25

Structural Determination of Agp1, a Phytochrome, *via* Surface Engineering. Soshichiro Nagano, Patrick Scheerer, Kristina Zubow, Katsuhiko Inomata, Tilman Lamparter, Norbert Krauss.

S-26

A Regulatory Membrane Protein Complex: The Sarcoplipin-bound Ca^{2+} -ATPase. Maike Bublitz, Anne-Marie L. Winther, Jesper L. Karlsen, Jesper V. MÅller, John B. Hansen, Poul Nissen, Morten J. Buch-Pedersen.

S-28

Protein Fold That uses Adhesion to an Internal Water Network. Tianjun Sun, Feng-Hsu Lin, Robert Campbell, John Allingham, Peter Davies.

S-29

Ca^{2+} is Needed for the Fold of a Novel β -Sandwich Extender Domain Found in a Bacterial Ice-binding Adhesin. Shuaiqi Guo,

Chris Garnham, Sarathy Karunan Partha, Tyler Vance, Robert Campbell, John Allingham, Peter Davies.

S-30

The Structure of the DNA-packaging Terminase pUL15 Nuclease Domain from the Prototypic Herpes Simplex Virus Type I. Liang Tang, Sundaresan Selvarajan Sigamani, Haiyan Zhao, Yvonne Kamau, Joel Baines.

S-31

Targeting UDP-galactopyranose Mutase: A Key Enzyme in Galf Biosynthesis. Richa Dhatwalia, Harkewal Singh, Michelle Oppenheimer, Pablo Sobrado, John Tanner.

S-32

Development of Novel Antitrypanosomatid Drugs Based on the Structure of Dihydroorotate Dehydrogenase. M. Cristina Nonato, .

S-33

Structures of the Bacteriophage Sf6 DNA-Packaging Terminase. Haiyan Zhao, Theodore Christensen, Yvonne Kamau, Liang Tang.

S-34

Evolution of a New Fold- the Structure of Cyanuric Acid Hydrolase. Tom Peat, Janet Newman, Sahil Balotra, Matthew Wilding, Santosh Panjekar, Nathan Cowieson, James Holton, Colin Scott.

S-35

Investigation of the Crystal Structure of Nature Goethite. Anton Chuev, Nikolai Fedorchuk.

S-36

Divergent Sequence Tunes Ligand Sensitivity in Phospholipid-Regulated Hormone Receptors. Paul Musille, Manish Pathak, Janelle Lauer, Patrick Griffin, Eric Ortlund.

S-37

The Structure of Bovine Parvovirus-1, an Infectious Pathogen of Young Calves. Shweta Kailasan, Brittany Gurda, Sujata Halder, Robert McKenna, Kevin Brown, Mavis Agbandje-McKenna.

S-38

X-ray Crystallographic Analysis of β -Carbonic Anhydrase from *P. aeruginosa*. Melissa Pinnard, Shalaka R. Lotlikar, Marianna A. Pa-trauchan, Robert McKenna.

S-39

The X-ray Crystal Structure of Human Aminopeptidase N Reveals a Novel Dimer And the Basis for Peptide Processing. Alan Wong, Dongxia Zhou, James Rini.

S-40

Regulation of the Quinone Reductase 2 Flavin Redox Switch Function by Casein Kinase 2 Inhibitors. Kevin Leung, Brian Shilton.

S-41

Structure-based Design of Novel Inhibitors Targeting the CXCL12 Chemokine. Emmanuel Smith, Brian Volkman, Joshua Ziarek, Francis Peterson, Rongshi Li, Yu Chen.

S-42

Structural Insights into the Mutations in α -L-Iduronidase that Cause Mucopolysaccharidosis Type 1 (MPS-1). Michael James, Haiying Bie, Jiang Yin, Xu He, Allison Kermod.

S-43

Structural Studies of GATA4 DNA Binding Domain. Eric Nezerwa, Mohammed Taha, Hyun-Joo Nam.

S-44

Crystallization and Preliminary Structure Determination of Self-Assembling Peptides in 3-D DNA Nanostructures. Kimberly N Rendek, Iosifina Sarrou, Jesse Bergkamp, Ingo Grotjohann, Raimund Fromme, Devens Gust, Petra Fromme.

S-45

Molecular Basis of Survivin Recognition of Two Histone Code Marks to Spatially Define the Inner Centromere of Mitotic Chromosomes. Ewa Niedzialkowska, Todd Stukenberg, Wlodek Minor.

Posters-S

S-46

Structure of MARK4 with a Pyrazolopyrimidine Inhibitor. Joseph Myers, Sophie Wu, John Newitt, Susan Kiefer, Chunhong Yan, Mian Gao, John Sack.

S-47

Structure Related Trypsin Cleavage of Peptides. Eva Tesarova, Tereza Slechtova, Kveta Kalikova, Martin Gilar, Juraj Sevcik.

S-48

Elucidating BRCT Structure and Biology. Jaime Davis, Jung Byun, Kevin Gardner.

S-49

Crystal Structure of Human Cytosolic Aspartyl-tRNA Synthetase, a Component of Multi-tRNA Synthetase Complex. Kyung Rok Kim, Sang Ho Park, Hyoun Sook Kim, Kyung Hee Rhee, Byung-Gyu Kim, Dae Gyu Kim, Mi Seul Park, Hyun-Jung Kim, Sunghoon Kim, Byung Woo Han.

S-50

Only with a Synchrotron: Understanding the Thermodynamics of Tris⁺ Flurbiprofen polymorphs. Carl H. Schwalbe, Miren Ramirez, Barbara R. Conway, Peter Timmins.

S-51

The New wwPDB Deposition and Annotation System. John Westbrook, Helen Berman, Gerard Kleywegt, John Markley, Haruki Nakamura.

S-52

Structure-based Identification of a Substrate Recognition Motif in HAD Phosphatase. Kyeong Kyu Kim, Tri Duc Ngo, Binh Le, Chi My Nguyen, Hyun Sook Lee, Hye-Yeon Hwang.

S-53

Molecular Insights into Neutrophilic Migration Revealed by the Structure of the Chemokine Receptor CXCR2 in Complex with the 1st PDZ Domain of NHERF1. Yuanyuan Jiang, Guorong Lu, Yanning Wu, Joseph Brun-

zelle, Chunying Li, Zhe Yang.

S-54

Enzyme Discovery for Natural Product Biosynthesis. George Phillips, Jr, Weijun Xu, David J Aceti, Craig A Bingman, Aram Chang, Sherif Elshahawi, Kate E Helmich, Jeremy R Lohman, Ming Ma, John G Primm, Ben Shen, Shanteri Singh, Michael G Thomas, Jon S Thorson, Donna M Troestler, Fengbin Wang, Rebecca Weerth, Ragothaman M Yennamalli.

S-55

Structural Analysis of Dihydropicolinate Reductase from *Vibrio vulnificus*. Nicholas Mank, Amy Arnette, Lesa Offermann, Maksymilian Chruszcz.

S-56

Using Crystal Structures, Mutagenesis and Inhibitors to Understand Allosteric Inhibition of a Key Bacterial Enzyme. David Sanders, Cuyler Conly, Yulia Skovpen, David Palmer.

S-57

Novel Bisphosphonate Inhibitors of Human Farnesyl Pyrophosphate Synthase with a Dual Mechanism of Action. Jaeok Park, Joris W De Schutter, Chun Y Leung, Youla S Tsantrizos, Albert M Berghuis.

S-58

Structural Analysis of Complexes Formed by the Major House Dust Mite Allergen Der p 1 with 5H8 and 10B9 Antibodies. Tomasz Osinski, Anna Pomas, Karolina Majorek, Jill Glesner, Lisa Vailes, Martin Chapman, Wladek Minor, Maksymilian Chruszcz.

S-59

Toward a Structure of the Membrane-Bound Cytochrome P450 2A1-Adrenodoxin Complex. Kimberly Hartfield, Andrew Annalora, David Stout.

S-60

Structure-based Drug Design of Inhibitors of the *Yersinia Pestis* Protein Tyrosine Phosphatase YopH. George Lountos, Medhanit Bahta, Scott Cherry, Joseph Tropea, Robert Ulrich,

Terrence Burke Jr., David Waugh.

S-61

Homology Models of Two BAHD Acetyl-Transferase Enzymes Important in Lignin Biosynthesis and Altered Lignin Composition. Kate Helmich, Saunia Withers, Curtis G. Wilkerson, John Ralph, George N. Phillips Jr.

S-62

Understanding the Mechanism and Substrate Profile of Baeyer-Villiger Monooxygenases using Crystallographic and Solution Techniques. Brahm Yachnin, Michelle B. McEvoy, Peter C. K. Lau, Albert M. Berghuis.

S-63

A Good Practice towards Effective UV Imaging of a Crystallization Experiment. Jian Xu, Scott Vaughan.

S-64

Crystal Structure and SAXS Modelling of the Bifunctional Antibiotic Resistance Enzyme AAC(6')-Ie/APH(2'')-Ia. Shane Caldwell, Albert Berghuis.

S-65

Crystallization and Characterization of Peptide Segments from the Amyloidogenic Protein, α -synuclein. Elizabeth Guenther, Magdalena Ivanova, David Eisenberg.

S-66

Construction of Antigen Specific Variable Lymphocyte Receptor (VLR) Libraries and Structure Determination of a VLR from Constructed Libraries. InWha Baek, Jang Mi Baek, Byung Woo Han.

S-67

Identification of Essential Residues Involved in Substrate Binding in Zea Mays Family GH19 Chitinase by Molecular Modeling and Kinetic Studies. Marcia Chaudet, Todd A. Naumann, Neil P.J. Price, David R. Rose.

S-68

Crystal Structure of Decaprenylphosphoryl-b-D-ribose 2'-epimerase from *Mycobacterium*

smegmatis. Hua Li, Gerwald Jogl.

S-69

Structure Solution of GPCRs with Low Sequence Identity to Known Structures. Gye Won Han, Fai Yiu Siu, Chong Wang, Qingping Xu, Vadim Cherezov, Raymond C. Stevens.

S-70

Discovery of Inhibitors of the Sos-mediated Activation of K-Ras. Qi Sun, Jason Phan, Michael Burns, Anders Friberg, Jason Burke, Edward Olejniczak, Alex Waterson, Taekyu Lee, Olivia Rossanese, Stephen Fesik.

S-71

Structures of RNA Polymerase-VPg-RNA Ternary Complexes and Insight into a Novel Role of VPg in Norovirus RNA Replication. Lee Ji-Hye, Park Beom Seok, Alam Intekhab, Han Kang Rok, Kim Sella, Seok Jong Hyeon, Kim Homin, Yang Jai Myung, Chung Mi Sook, Kim Kyung Hyun.

S-72

A New Approach Towards Damage-free and High-resolution Protein Crystallography at SACLA. Kunio Hirata, Kunio Hirata1, Go Ueno, Hironori Murakami, Masaki Yamamoto, Takehiko Tosha, Tamao Hisano, Minoru Kubo, Hiroshi Sugimoto, Yoshitsugu Shiro, Hideo Ago, Eiki Yamashita, Jian-Ren Shen, Kyoko Shinzawa-Ito, Koji Kato, Miki Hatanaka, Shuhei Takemura, Naomine Yano, Takashi Ogura, Shinya Yoshikawa, Tomitake Tsukihara.

S-73

Insights into Iron Uptake Mechanism in Ferritin from *Helicobacter pylori*. Sella Kim, Yi-Ho Park, Ji Hun Yang, Ki Joon Cho, Ji-Hye Lee, Cheolju Lee, Mi Sook Chung, Kyung Hyun Kim.

S-74

Apo-Structure of TDP-Rhamnose 3'-O-Methyltransferase(CalS11), An Enzyme in Calicheamicin Biosynthesis. Lu Han, Shanteri Singh, Jon Thorson, George Phillips.

Posters-S

S-75

Innovation in Thin-Film Crystal Mounts for use in Concurrent Visualization, Diffraction and Spectroscopy. Benjamin Apker, Di Qian, Robert Thorne.

S-76

Structural and Functional Analyses of the Interactions Between USP7-NTD and E2 Conjugating Enzymes. Leila Ashurov, Anthony La Delfa, Majda Mohamed, Yi Sheng, Vivian Saridakis.

S-77

Methods for Phasing of Coherent Diffraction Patterns from Variable Size Nanocrystals. Richard Bean, Richard Kirian, Kenneth Bereylein, Miriam Bartelmess, Oleksandr Yefanov, Andrew Martin, Alejandro Cmara, Haiguang Liu, John Spence, Henry Chapman.

S-79

Crystalline Formulation of a Sclerostin Antibody Increases Bone Mineral Density in Rats. Twinkle Christian, Christi Clogston, Theingi Thway, Vibha Jawa, Kelly Warmington, Xiaodong Li, Chris Paszty, Timothy Osslund.

S-80

Unusual Structural Malleability of the N-terminal Domain of the p90 Ribosomal Ser/Thr Kinase RSK2: Implications for Drug Design. Zygmunt Derewenda, Darkhan Utepbergenov, Urszula Derewenda.

S-81

Studies of Active Pharmaceutical Ingredients and Derivatives using Synchrotron Radiation. Graciela Diaz de Delgado, Robert Toro, Luis Len, Julio Trejo, Jose Miguel Delgado, Chun-Hsing Chen, Maren Pink.

S-82

Structural Studies on Membrane Protein Complexes. Pascal Egea, Andrew Ah Young, Cedric Eichmann, Antoine Koehl, Mindy Peng.

S-83

Impact of Crystal Morphology to Bulk Pow-

der Properties of Active Pharmaceutical Ingredients. Qi Gao, Joshua Engstrom, Daniel Roberts, Chenkou Wei, Jonathan Brown, Chijien Lai.

S-84

Structural Characterization of (anti)-4-cyclohexyl-5-vinylloxazolidin-2-one. Danielle Gray, Rulin Ma, Thomas J. Osberger, M. Christina White.

S-85

Structure of Family 31 Glycoside Hydrolase Yici: Insights Into Sucrase-Isomaltase and Maltase-Glucoamylase. Kyra Jones, Warren Wakarchuk, David Rose.

S-86

Structural Studies Between USP7-NTD and its Substrates. Niharika Luthra, Anthony La Delfa, Vivian Saridakis.

S-87

Ferrous Iron Binding and Oxidation by Ferritin from a Pennate Diatom. Michael Murphy, Stephanie Pfaffen.

S-88

Linking Structure and Function in Finite Materials. Katharine Page, Kevin Baldwin, Joseph Peterson, Heinz Nakotte.

S-89

Generating the Chemical Complexity of Tubulin: Insights from Crystal Structures of Tubulin Post-Translational Modification Enzymes. Antonina Roll-Mecak.

S-90

An Analysis on Role of Type I Copper Protein Amicyanin Mutants on Electron Transfer. Narayanasami Sukumar, M. Choi, V.L. Davidson.

S-91

Using a Commodity 3D HDTV for Collaborative Structural Biology. Ragothaman Yennamalli, Raj Arangarasan, Aaron Bryden, Michael Gleicher, George N Phillips Jr.

S-93

Rastering Tools Make Successful Data Collection from Challenging Samples Possible. Ruslan Sanishvili, Mark Hilgart, Sudhir Babu Pothineni, Shenglan Xu, Rui Wu, Dali Liu, Michael Becker, Venugopalan Nagarajan, Sergey Stepanov, Craig Ogata, Janet Smith, Robert Fischetti.

S-94

Structural and Functional Characterization of *Campylobacter jejuni* Ferric Uptake Regulator (CjFur). Sabina Sarvan, James Butcher, Alain Stintzi, Jean-Francois Couture.

S-95

Structural Insights into the Substrate Specificity of a 6-Phospho- β -glucosidase BglA-2 from *Streptococcus pneumoniae*. Yong-Liang Jiang, Wei-Li Yu, Andreas Pikis, Wang Cheng, Xiao-Hui Bai, Yan-Min Ren, John Thompson, Cong-Zhao Zhou, Yuxing Chen.

S-96

Test Samples for Measurements in the Nanometer Range. Boris Kodess, Paul Kodess.

S-98

Elucidating the Mechanism of Inhibition of Phosphoenolpyruvate Carboxykinase by 3-mercaptopycolinic Acid. William Lotosky, Marc Balan, Troy Johnson, Todd Holyoak.

S-99

Structural Insights into the Isavirus Entry Mechanism. Jonathan D Cook, Hazel Soto-Montoya, Jeffrey E. Lee.

S-100

Structural Insights into Superantigenic T Cell Activation. Karin Rodstrom, Karin Lindkvist-Petersson.

S-101

A Structural Biology Approach in Studying Protein Evolution and Functional Diversification. Dinesh Christendat.

S-102

Crystal Structure of PKC-Related Kinase 1 (PRK1). Philip Chamberlain, Afshin Mahmoudi, Barbra Pagarigan, Mahan Abbassian, Pilgrim Jackson, Brian Cathers.

S-103

Texture Analysis of Complex Geomaterials: A TOF Neutron Diffraction Approach. Juan Gomez Barreiro, Jose Manuel Benitez Perez, Marco Voltolini, Hans-Rudolf Wenk, Sven Vogel, Jose Ramon Martinez Catalan, Icaro Frois Dias da Silva, Pedro Castiñeiras, Laura Gonzalez Fernandez.

Monday Posters

M-01

Three Porous Metal Organic Frameworks Based on a Rigid Tricarboxylic Ligand. Yao Chen, Shengqian Ma.

M-02

A Few Handy Tools for Monitoring Data Quality On-the-Fly. Zheng-Qing Fu, John Rose, John Chrzas, Bi-Cheng Wang.

M-03

A Flavin N(5)-Adduct Provides Insight into the Catalytic Mechanism of Rv1346, an Acyl-ACP Dehydrogenase from *Mycobacterium tuberculosis*. Ai Fen Chai, Jodie Johnston, Esther Bulloch, Genevieve Evans, Shaun Lott, Edward Baker.

M-04

A Mechanochromic Metal Salt that Turns on Vapochromic Behavior. Amie Norton, Jeanette Krause, William Connick.

M-05

A Novel Approach of Crystal-Quality Improvement by "The Multi-Step Soaking Method". Miki Senda, Takeru Hayashi, Masanori Hatakeyama, Toshiya Senda.

M-06

Acetylation of the N-terminus of Sir3 Stabilizes the Interaction Between Sir3 BAH Domain

Posters-M

and Nucleosome. Na Yang, Dongxue Yang, Qianglin Fang, Mingzhu Wang, Rui-Ming Xu.

M-07

Active Site Structural Flexibility of β -L-fucosidase GH29 from *Fusarium graminearum* Revealed by X-ray Crystallography. Hongnan Cao, Jonathan Walton, Phil Brumm, George N Phillips Jr., Great Lakes Bioenergy Research Center.

M-08

An Insight into the Fundamental Process of Nucleation for Organic Molecules: p-Aminobenzoic Acid and Benzoic Acid. Rachel Sullivan, Roger Davey.

M-09

Application of DIALS and CCTBX Software Towards Real-time Processing of Diffraction Data at the Terabyte Scale. Aaron Brewster, Johan Hattne, Richard Gildea, Nicholas Sauter.

M-10

Assignment of Oxidation States in the Nitrogenase Metal Centers by Crystallographic Studies at Multiple X-ray Wavelengths. Thomas Spatzal, Douglas C. Rees.

M-12

Conformations of 2-Methyl-2,4-Pentanediol in Protein Crystals. Dahniel Sastow, Ariel Axelbaum, Jean Jakoncic, Jerome Karp, Sergey Buldyrev, Bruce Hrnjez, Neer Asherie.

M-13

Crystal Engineering Charge Transfer Complexes of Phenothiazine with Various Electron Acceptor Molecules. Sanaz Khorasani, Manuel Fernandes.

M-14

Crystal Structure and Function Assignment of Conserved Protein TM1086 from *Thermotoga maritima*. Marcin Domagalski, Igor A. Shumilin, Jing Hou, Karolina L. Tkaczuk, Maksymilian Chruszcz, Wladek Minor.

M-15

Crystal Structure of 1-(6-chloro-1-methyl-1H-imidazo [4,5-c]pyridin-4-yl)-3-(2-chlorophenyl)urea. M. Vinduvahini, H.C. Devarajegowda.

M-16

Crystal Structure of 5-{4'-(5-Benzyl-2H-tetrazol-2-yl) methyl} biphenyl-2-yl}-1H-tetrazole. H.C. Devarajegowda.

M-17

Crystal Structure of CagA, an Oncoprotein from *Helicobacter pylori*. Toshiya Senda, Takeru Hayashi, Miki Senda, Masanori Hatakeyama.

M-18

Crystal Structure of Human APOBEC3C and HIV-1 Vif-binding Interface. Shingo Kitamura, Hiroataka Ode, Masaaki Nakashima, Mayumi Imahashi, Yuriko Naganawa, Yoshiyuki Yokomaku, Nobuhisa Watanabe, Atsuo Suzuki, Wataru Sugiura, Yasumasa Iwatani.

M-19

Crystal Structure of Human Apoptosis Inhibitor 5 Reveals Protein-Protein Interaction Module. Byung Il Lee.

M-20

Crystal Structure of Human DSP21, a Member of the Mitochondrial Dual-specific Phosphatase. Daegwin Jeong, Tae-Sung Yoon.

M-21

Crystal Structure of Mutant D68N Archaeal Inorganic Pyrophosphatase at 1.5Å: A Preliminary Analysis of an Active Site Variant. Manavalan Gajapathy, Manavalan Gajapathy, Ronny Hughes, Joseph Ng.

M-22

Crystal Structure of N-(6-chloro-1-methyl-1H-imidazo [4,5-c]pyridin-4-yl)benzenesulfonamide. J. Shylajakumari, H.C. Devarajegowda.

M-23

Crystal Structure of *Schistosoma Mansoni* Adenylosuccinate Lyase in Complex with AMP. Larissa Romanello, Juliana Torini, Louise Bird, Joanne Nettleship, Raymond Owens, Yamini Reddivari, Jose Brandao-Neto, Humberto D'Muniz Pereira.

M-24

Crystal Structures of *Saccharomyces cerevisiae* D-arabinose Dehydrogenase Ara1 and its Complex with NADPH: Implication for NADPH and Substrate Recognition. Weifang Li, Cong-Zhao Zhou.

M-25

Crystal Structures of the Peripheral Membrane Flavoprotein Proline Utilization A: Gated Substrate Channeling And Quinone Binding. Harkewal Singh, John Tanner.

M-26

Crystallization of an Influenza Nucleoprotein-RNA Complex. Robert Kirchdoerfer, Ian Wilson.

M-27

Crystallization of Lysozyme with (R)-, (S)- and (RS)-2-methyl-2,4-pentanediol. Ariel Axelbaum, Jean Jakoncic, Mark Stauber, Jacob Berger, Neer Asherie.

M-28

Diamond Crystal - Fast Self-Healing and High Temperature Nuclear Material. Boris Udovic.

M-29

Differential Temperature Dependence of Tobacco Etch Virus and Rhinovirus 3C Proteases. David Waugh, Sreejith Raran-Kurussi, Jozsef Tozser, Scott Cherry, Joseph Tropea.

M-30

Differentiation of Oxide and Fluoride Anions with Single Crystal, Laboratory X-Ray Diffraction. Martin D. Donakowski, Kenneth R. Poeppelmeier.

M-31

Diversity in a Common Framework: Oddities in the Quaternary Structures of LysR-Type Transcriptional Regulators. Cory Momany, Melesse Nune, Ellen Neidle.

M-32

Dual Function of Pol Gamma in Mitochondrial DNA Replication and Repair. Whitney Yin, Kutzneysov, Christle Shumate, Young-Sam Lee, Eric Meng.

M-33

Energy Dependence of Radiation Damage. Dorothee Liebschner, Gerd Rosenbaum, Zbigniew Dauter.

M-34

Fullerene Fragments as Ideal Hosts for C60 and C70-Fullerenes. Marina A. Petrukhina, Michael V. Ferguson, Sarah N. Spisak, Alexander S. Filatov, Charles Campana, Evgeny V. Dikarev.

M-35

GPCR Network - Structure and Function of GPCRs Through Open Collaborations. Enrique Abola, Ruben Abagyan, Vadim Cherezov, Said Eshaghi, Tracy Handel, Vsevolod Katritch, Peter Kuhn, Hugh Rosen, Kurt Wuthrich, Raymond Stevens.

M-36

Head Hunting: Targeting the Influenza Hemagglutinin Receptor Binding Site. Peter Lee, Ayato Takada, James Crowe, Jr., Yoshikazu Kurosawa, Ian Wilson.

M-37

High-pressure-induced Phase Transition of Protein Crystals. Hiroyuki Yamada, Takayuki Nagae, Nobuhisa Watanabe.

M-38

Human Asparaginase 3: Structural Insights into Glycine-Accelerated Enzyme Activation and Substrate Hydrolysis. Julian Nomme, Ying Su, Christos Karamitros, Theresa McSorley, Manfred Konrad, Arnon Lavie.

Posters-M

M-39

Hydronium Ions and Protonation States in Reduced and Oxidized Forms of *Pyrococcus furiosus* Rubredoxin. Maxime Cuypers, Sax Mason, Edward Mitchell, Matthew Blakeley, Michael Haertlein, Trevor Forsyth.

M-40

In-vivo Crystallization and XFEL Techniques: the New Next-of-kin of “Crystallography Plates and 3rd Generation Synchrotrons. Francois-Xavier Gallat, Daisuke Tsuji, Tetsuya Higashi, Kohji Itoh, Leonard M.G. Chavas.

M-41

Visualizing the Tetrahedral Transition State in the Catalytic Mechanism of Hydrolases with an Arsenic Substrate Analogue by the Example of the Crystal Structure of the Esterase egHle. Christine Tolzer, Sonia Pal, Hilde Watzlawick, Josef Altenbuchner, Karsten Niefind.

M-42

Long Wavelength and Multicrystal Data Collection at the Australian Synchrotron. Christine Gee, Tom Peat, Janet Newman, James Holton, David Aragao, Rachel Williamson, Alan Riboldi-Tunncliffe, Nathan Cowieson, Santosh Panjekar, Tom Caradoc-Davies.

M-43

Malaria Parasite Invasion of Red Blood Cells: Receptor Recognition and Antibody Inhibition. Niraj Tolla, Joseph Batchelor, Brian Malpede, Edwin Chen, Daniel Lin, Nichole Salinas, May Paing.

M-44

Mechanistic Insights Revealed by the Crystal Structures of the Nucleotide-Bound PI5P4K II β . Yu-Hua Lo, Koh Takeuchi, Miki Senda, Ichio Shimada, Lewis C. Cantley, Atsuo T. Sasaki, Toshiya Senda.

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Study of PFSA Ionomers using X-ray Scattering Techniques. Ahmet Kusoglu, Adam

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The Crystal Chemistry and Enantiomer Separation of the Triazolylketone, 1-(4-chlorophenyl)-4,4-dimethyl-2-(1H-1,2,4-triazol-1-yl)pentan-3-one (TAK). Ghazala Sadiq, Roger Davey, Colin Seaton.

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High Performance Computing for GISAXS. Alexander Hexemer, Sherry Li, Slim Chourou, Abhinav Sarje.

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X-ray Structural Study of New Acentric Co-crystals for Industrial Applications. Sergiu Draguta, Evghenia Leonova, Marina Fonari, Tatiana V. Timofeeva.

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G-Rob: a Fully Robotized Crystallography Setup Developed on Beamline FIP- BM30A at the ESRF. Jean-Luc Ferrer, Xavier Vernede, Yaser Heidari, Nathalie Larive, Michel Pirocchi, Yoann Sallaz-Damaz, Maxime Terrien, Christophe Berzin, Pierrick Rogues, Franck Borel.

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Challenges and Solutions for Enabling Facebook-like Graph-search on Small and Macro-molecular Structural Data. Talapady Bhat, John Elliott, Carelyn Campbell, Ursula Kattner, Shir Boger, Anne Plant.

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Immune Recognition of HIV-1 and Implications for Vaccine Design. Ian A. Wilson.

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SCrALS: Bright Light, Micro Crystals, Great Structures. Allen Oliver, Jeanette Krause.

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Studies in Useful Hard X-ray Induced Chemistry. Michael Pravica, Ligang Bai, Daniel Sneed, Quinlan Smith, Changyong Park.

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mosquito® Crystal and mosquito® LCP: Fast, Reliable Automation of Protein Crystallisation Drop Set-up. Soheila Vaezeslami, Joby Jenkins, Wendy Gaisford, David Smith.

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Structural and Functional Insights into (S)-Ureidoglycine Aminohydrolase, Key Enzyme of Purine Catabolism in *Arabidopsis thaliana*. Sangkee Rhee, Inchul Shin, Riccardo Percudani.

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Just Not Your Protein: Where Horror Story and Reality Meet. Kay Perry, Jonathan Schuermann.

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Crystal Structures of Group 2 Citrate Salts. James Kaduk.

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Integration of CBF, NeXus and HDF5. Herbert J. Bernstein, Jonathan M. Sloan, Graeme Winter, Tobias S. Richter, NeXus International Advisory Committee, Committee on the Maintenance of the CIF Standard.

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Structural Insights into a New Type of Pili from the Human Gut Microbiome. Qingping Xu, Mikio Shoji, Hsiu-Ju Chiu, Lukasz Jaroszewski, Mark W. Knuth, Marc-Andre Elslinger, Ashley M. Deacon, Adam Godzik, Koji Nakayama, Ian A. Wilson.

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Solid State Characterization of a New Salt of Mebendazole: Mebendazole mesylate Monohydrate. Karina de Paula, Geraldo Cami, Elena Brusau, Griselda Narda, Javier Ellena.

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Insights into the Structure of a New Salt of Isoniazid Drug: Isoniazid Nitrate. Cristiane Cabral de Melo, Javier Ellena.

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Anti-HIV-1 Neutralizing Antibody 2g12 in Complex with Bacterial Oligosaccharide. Robyn Stanfield, B.E. Clark, K. Auyeung, E. Fregolino, C. De Castro, R. Pantophlet, I.A. Wilson.

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The Crystal Structure of cGMP Dependent Protein Kinase II/Rab11b Complex Reveals The Molecular Details for GKIP-PKG Interaction. Albert Reger, Matthew Yang, Elaine Guo, Darren Casteel, Choel Kim.

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SSGCID: Activity Based Protein Profiling and X-ray Crystallography Establish a New RNase Family in Actinobacteria. James Fairman, Jan Abendroth, Anja Ollodart, Emma X, Peter Myler, Thomas Edwards, Vickery Arcus, Christoph Grundner.

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Targeting the Biosynthesis of the Cell Wall of *Mycobacterium tuberculosis*. Mario Bianchet, Sabri B Erdemli, Radhika Gupta, William R Bishai, Gyannu Lamichhane, Mario Amzel.

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Upgrade Program of Structural Biology Beamlines at the Photon Factory. Yusuke Yamada, Naohiro Matsugaki, Leonard M.G. Chavas, Masahiko Hiraki, Nobutaka Shimizu, Noriyuki Igarashi, Soichi Wakatsuki, Toshiya Senda.

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Structural Characterization of *Pandoraea pnomenusa* B-356 Biphenyl Dioxygenase Reveals Features of Potent PCB-Degrading Enzymes. Christopher Colbert, Nathalie Agar, Pravindra Kumar, Justin Polowski, Lindsay Eltis, Jeffrey Bolin.

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Crystal Structure of Tandem ACT Domain-Containing Protein ACTP from *Galdieria sulphuraria*. Byung Woo Han, Eduard Bitto, Do Jin Kim, Craig Bingman, Hyun-Jung Kim, George Phillips.

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Crystal Structure of the Fluorescence Recovery Protein (FRP) Involved in Cyanobacterial Photoprotection and Identification of its Active Site. Markus Sutter, Adja Wilson, Ryan Leverenz, Rocio Lopez Igual, Adrien Thurotte, Annette Salmeen, Diana Kirilovsky, Cheryl Kerfeld.

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JCSG Top96: A Rationally Designed Crystallization Screen Based on over 1000 Deposited Protein Structures from the Joint Center for Structural Genomics. Marc C. Deller, Tom Clayton, Marc A. Elslinger, Scott A. Lesley, Ian A. Wilson.

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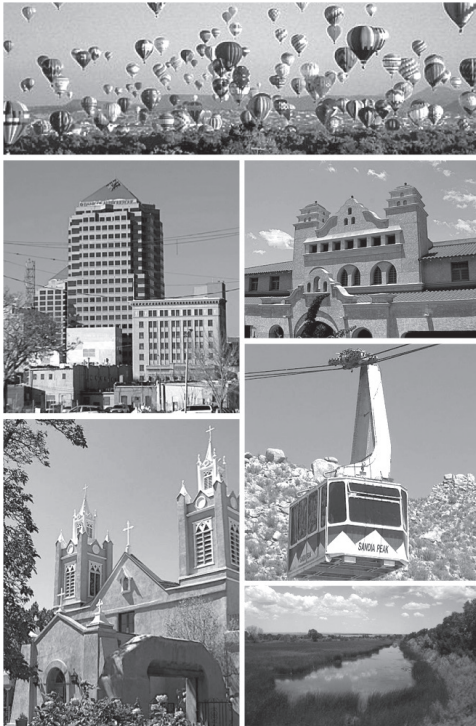
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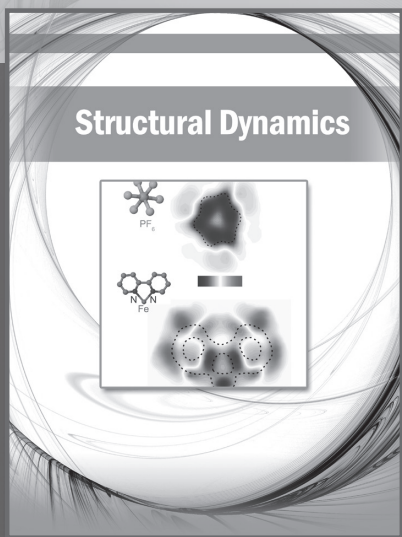
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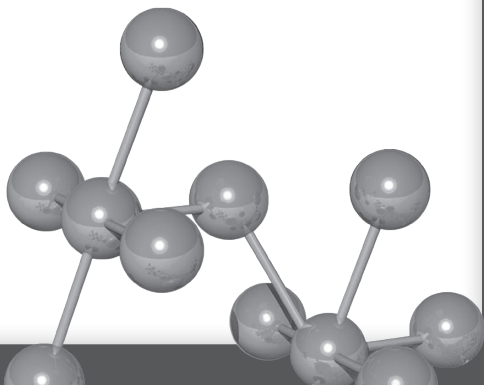
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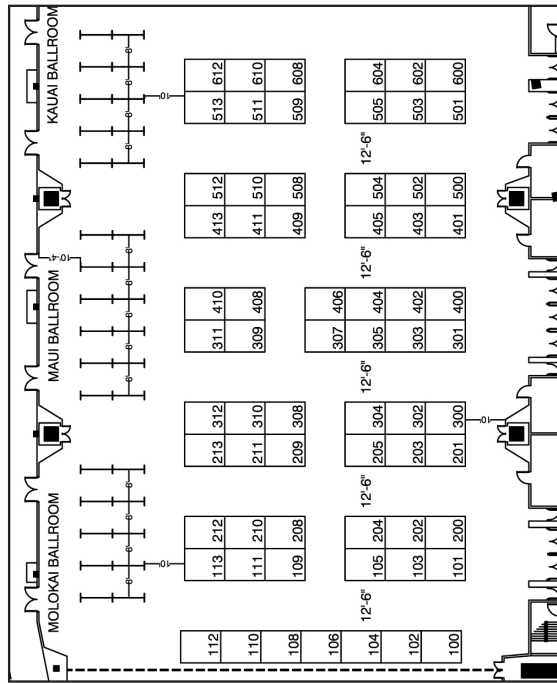
Program at a Glance

Morning		Afternoon		Evening	
Saturday July 20	<p>WK.01 Biological SAXS-Theory & Practice Track A Honolulu/Kahuku</p> <p>WK.01 Biological SAXS-Theory & Practice Track B Oahu/Waiialua</p> <p>WK.02 Introduction to the GSAS Waianae</p> <p>WK.03 Get the Most out of CSDS Kohala/Kona</p>	<p>WK.01 Biological SAXS-Theory & Practice Track A Honolulu/Kahuku</p> <p>WK.01 Biological SAXS-Theory & Practice Track B Oahu/Waiialua</p> <p>WK.02 Introduction to the GSAS Waianae</p> <p>WK.03 Get the Most out of CSDS Kohala/Kona</p>	<p>TR.02 Transactions Symposium (II) Lanai</p> <p>03.01 Supramolecular Assemblies Lanai</p> <p>13.04 General Interest (I) Honolulu/Kahuku</p> <p>09.01 Nanomaterial Structure from Diffraction Data (II) Oahu/Waiialua</p> <p>11.02 Experimental Advances Waianae</p> <p>11.02 Dynamic & Flexible Structures in Biomolecules (I) Kohala/Kona</p> <p>11.02 Femtosecond X-ray Pulses: Tools for Crystallography Kohala/Kona</p>	<p>New Attendee/Student Orientation 5:30pm Kohala/Kona</p> <p>Opening Reception and Exhibit Show 7:30pm Ballroom</p>	
Sunday July 21	<p>AW.01 Bau Award Lecture-Thomas Koetzie Lanai</p> <p>TR.01 Transactions Symposium (I) Small Angle Scattering Honolulu/Kahuku</p> <p>13.01 Structural Enzymology (I) Lanai</p> <p>13.02 Nanomaterial Structure from Diffraction Data (I) Oahu/Waiialua</p> <p>13.03 Theory and Modeling Improving Structural Models through Computational Tips & Tricks Waianae</p> <p>11.01 Multi-crystal & Micro-crystal Data Collection Kohala/Kona</p>	<p>TR.02 Transactions Symposium (II) Lanai</p> <p>03.01 Supramolecular Assemblies Lanai</p> <p>13.04 General Interest (I) Honolulu/Kahuku</p> <p>09.01 Nanomaterial Structure from Diffraction Data (II) Oahu/Waiialua</p> <p>11.02 Experimental Advances Waianae</p> <p>11.02 Dynamic & Flexible Structures in Biomolecules (I) Kohala/Kona</p> <p>11.02 Femtosecond X-ray Pulses: Tools for Crystallography Kohala/Kona</p>	<p>12.01 Career Odyssey Panel Oahu/Waiialua</p> <p>Poster Session S 5:30pm Ballroom</p> <p>YSSIG Mixer (ticket required) 8:00pm Princess Hotel</p> <p style="text-align: center;"><u>SIG MEETINGS</u></p> <p>Sm Angle Scattering 12:00pm Honolulu/Kahuku</p> <p>Fiber Diffraction 12:00pm Kohala/Kona</p> <p>Joint Service & Sm Molecule 12:00pm Waianae</p> <p>BioMac 5:00pm Lanai</p> <p>General Interest 5:00pm Honolulu/Kahuku</p>		
Monday July 22	<p>AW.02 Fankuchen Award Lecture-Alex McPherson Lanai</p> <p>13.05 Structure Validation Lanai</p> <p>13.06 Cool Structures Honolulu/Kahuku</p> <p>13.07 Materials for a Sustainable Future Oahu/Waiialua</p> <p>09.02 Nanostructured Thin Films - Frontiers of Grazing Incidence Scattering Waianae</p> <p>13.08 Building Protein and Small Molecule Research Capacity at an Undergraduate Institute Kohala/Kona</p>	<p>01.01 Structural Enzymology (II) Nucleotide Metabolism Modification & Interactions Lanai</p> <p>13.09 Materials for a Sustainable Future & Structure/ Function of Metal-Organic Frameworks Oahu/Waiialua</p> <p>09.01 Dynamic & Flexible Structures in Biomolecules (II) Waianae</p> <p>11.03 Femtosecond X-ray Pulses: Biological Applications Kohala/Kona</p> <p>10.01 Interplay of Crystallography, NMR and Theoretical Methods Honolulu/Kahuku</p>	<p>Poster Session M 5:30pm Ballroom</p> <p style="text-align: center;"><u>SIG MEETINGS</u></p> <p>YSSIG 12:00pm Lanai</p> <p>Industrial Kohala/Kona</p> <p>Canadian Div. Waianae</p> <p>Joint: Neutron/Materials/Powder 12:00pm Oahu/Waiialua</p> <p>Synchrotron Radiation 5:00pm Kohala/Kona</p>		
Tuesday July 23	<p>AW.03 Elter Early Career Award Lecture – Eric Oltlund Lanai</p> <p>TR.03 Transactions Symposium (III) Emerging Characterization Facilities & Tools Honolulu/Kahuku</p> <p>12.02 Elter Early Career Award Symposium Lanai</p> <p>13.10 Reviewer Practices-Engaging New Reviewer Practices-Engaging New Kohala/Kona</p> <p>09.03 Crystallographic Reviews Waianae</p> <p>13.11 Membrane Protein Scattering Complementary Methods in Crystals & in Solution (I) Oahu/Waiialua</p>	<p>TR.04 Transactions Symposium (IV) Chemical Crystallography Honolulu/Kahuku</p> <p>13.12 Structural Genomics for the Home Laboratory Lanai</p> <p>13.14 Materials Discovery Kohala/Kona</p> <p>13.11 Complementary Methods in Crystals & in Solution (II) Oahu/Waiialua</p> <p>13.15 Contemporary Crystal Engineering (I) Waianae</p>	<p>Association Business Meeting 5:00pm Kohala/Kona</p> <p>Poster Session T 5:30pm Ballroom</p> <p>13.21 Partnerships for Broader Crystallographic Data Accessibility 7:30pm Honolulu/Kahuku</p>		
Wednesday July 24	<p>AW.04 Trueblood Award Lecture – Thomas Terwilliger Lanai</p> <p>01.02 Host Pathogen Interactions Lanai</p> <p>11.04 Specialized MX Experiments Kohala/Kona</p> <p>13.15 Contemporary Crystal Engineering (II) Waianae</p> <p>03.02 General Interest (II) Honolulu/Kahuku</p> <p>13.17 Microstructural Evolution Oahu/Waiialua</p>	<p>13.18 Nanodomains & Beyond Waianae</p> <p>03.02 General Interest (III) Honolulu/Kahuku</p> <p>04.01 From Knowledge to Design: Data Mining in Materials Chemistry Oahu/Waiialua</p> <p>13.20 Exciting Structures Lanai</p>	<p>Annual Awards Banquet (ticket required) Royal Hawaiian Hotel Montaroch Room</p> <p>Cash Bar 6:30pm Dinner 7:30pm</p>		
Thursday July 25	<p>Planning Session for 2014 ACA Annual Meeting in Albuquerque, New Mexico 9:00 - 11:00am Kohala/Kona</p>	<p style="text-align: center;">2013 EXHIBIT SHOW</p> <p style="text-align: center;">Ballroom</p>	<p style="text-align: center;">2013 EXHIBIT SHOW</p> <p style="text-align: center;">Ballroom</p>	<p style="text-align: center;">Saturday, 7:30pm-10:30pm</p> <p style="text-align: center;">Sunday, Monday, Tuesday, 10:00am-7:30pm</p>	

2013 EXHIBIT SHOW Sheraton Hotel Ballroom

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

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Synchrotron Radiation Pete Dunten
Young Scientist Albert Reger

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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, a 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 2,000. National meetings are held annually. There are 12 Scientific Interest Groups (SIG) 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 to 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.