

WORKSHOPS

WK.01 Methods in Neutron Protein Crystallography

Paul Langan, langan_paul@lanl.gov

Paul Adams, pdadams@lbl.gov

The use of neutron protein crystallography is growing at the moment with the development of new beam lines and next generation neutron sources. This full-day workshop has two main objectives 1) to introduce protein crystallographers to the facilities available and experimental requirements for neutron crystallography 2) to teach people how to use macromolecular structure determination tools that are being developed by the consortium for Computation Tools for Neutron Protein Crystallography (CT for NPX). The workshop will precede a Transaction Symposium "The Future of Neutron Crystallography: Smaller Crystals, Larger (Macro) Molecules." Together the workshop and Transaction Symposium will provide a comprehensive introduction to those interesting in using neutron protein crystallography. The early morning talks will provide an overview of available facilities and methods for protein deuteration, crystal preparation and data collection. Talks will be given by leaders in these fields. The workshop will then focus on existing computer programs, including those developed by CT for NPX for structure refinement. CT for NPX is a NIH funded consortium that is contributing a computational workbench that structural biologists, with a range of crystallographic experience, can use alternatively for X-ray or neutron structure determination. Participants will be guided through the use of CNSsolve and PHENIX by members of the CT for NPX consortium including:

Paul Langan, Los Alamos Nat'l Lab

Paul Adams, Lawrence Berkeley Nat'l Lab

Marat Mustyakimov, Los Alamos Nat'l Lab

Pavel Afonine, Lawrence Berkeley Nat'l Lab

Leighton Coates, Los Alamos Nat'l Lab

These sessions will be organized into tutorials that guide the participants through examples of the application of each program to a real neutron structure refinement. The tutors will also make themselves available throughout the meeting for hands-on tutorials with workshop participants.

The workshop registration fee is \$80 for students, \$100 for all others and does not include breakfast or lunch.

WK.02 The Management of Synchrotron Image Data: The imgCIF File System and Beyond

Herbert J. Bernstein, yaya@dowling.edu

Robert M. Sweet, sweet@bnl.gov

The pace of data collection and the volume of data collected at synchrotron beam lines is increasing. The ACA Data, Standards, and Computing Committee is spearheading an effort to improve the efficiency of the handling and storage of these data by encouraging the adoption of common data formats and standard software interfaces. The goal of this is firstly to have the data be self defining, therefore equally accessible to all data-reduction and -visualization codes. The second goal, for the purposes of secure archiving, is to provide a robust internal documentation of the source of the data.

The first imgCIF/CBF workshop took place at the Brookhaven National Laboratory in 1997 and proposed a format combining support for an efficient binary representation of images with a fully CIF-compliant ASCII equivalent. An imgCIF/CBF dictionary, and software to support the format, were created, are available on the web, and are described in Volume G of the IUCr International Tables for Crystallography. Now the community should adopt a consensus standard for management of data at synchrotron beam lines, and to make it easier for users to process data taken from various beam lines. Also, as our science evolves, new concepts will be considered; possibilities include NeXuS and XML.

The primary activity at the first workshop will be to adopt a new standard for synchrotron image data for immediate use. As a practical matter, that standard should be based on the existing imgCIF IUCr standard. At the same time, the attendees, including standards developers, crystallographic software developers, and interested users, will be invited to seek a consensus on the next steps to extend imgCIF/CBF. A follow-up workshop will take place during the 2006-2007 academic year to resolve any issues that arise in the adoption of the adjusted imgCIF standard, to discuss the extensions, and to enhance the standard as appropriate. There will be a wrap-up workshop in summer 2007.

The workshop registration fee is \$80 for students, \$100 for all others, and does not include breakfast or lunch.

WK.03 An Introduction to Grazing Incidence Small Angle Scattering with X-rays and Neutrons

Jin Wang, wangj@aps.anl.gov

Randall Winans, rewinans@anl.gov

This half-day workshop will focus on the applications of GISAXS and GISANS, the current technical capabilities to support these applications, and most importantly, the challenges to advance this new technique, especially, in this new age of nanoscience and nanotechnology. To promote the science that can be facilitated with these techniques on nano to meso scales, we will hold a one-half day workshop. A preliminary list of speakers follows:

Gilles Renaud, CEA Grenoble

Peter Mueller-Buschbaum, Technical Univ. of Munich

Byeongdu Lee, Argonne National Lab

Ed Kramer, Univ. of California, Santa Barbara

The workshop registration fee is \$80 for students, \$100 for all others and does not include breakfast or lunch.

TR.01 Transactions Symposium: The Future of Neutron Crystallography: Smaller Crystals, Larger (Macro) Molecules

Robert Bau, bau@usc.edu

Paul Langan, langan_paul@lanl.gov

Thomas Koetzle, tkoetzle@anl.gov

Alberto Podjarny, podjarny@igbmc.u-strasbg.fr

This year's Transactions Symposium will feature a full-day program that will highlight the advances and future prospects in neutron crystallography and especially its applications to macromolecules. The program will include several overview talks that will provide a broad introduction to the field, including a survey of the instrumentation for neutron crystallography that is available and is planned at user facilities around the world. The results of recent experiments will be presented including neutron protein structures analyzed on BIX at JAERI (Ibaraki, Japan), LADI at ILL (Grenoble, France), and PCS at LANSCE (Los Alamos, New Mexico). Speakers will offer their visions of the exciting possibilities that will be realized with the next generation of powerful neutron sources: ISIS-TII, SNS, J-PARC, and (currently in the planning stage) NxGEN and the ESS.

Speakers:

Robert Bau, Univ. of Southern California

Nobuo Niimura, Ibaraki Univ., Japan

Alberto Podjarny, IGBMC, France

Arthur Schultz, Argonne National Lab

Lee Brammer, Univ. of Sheffield, UK

Gerald Bunick, Univ. of Tennessee

A workshop on "Methods in Neutron Protein Crystallography" is planned to precede the Transactions Symposium. Together the workshop and the Transactions Symposium will provide a comprehensive introduction to those interested in using neutron protein crystallography.

Biological Macromolecules SIG Sessions

01.01 New Structures

Stephan Ginell, ginell@anl.gov

David N. Garboczi, dgarboczi@niaid.nih.gov

This session will highlight recent macromolecular crystal structures of particular importance and interest to a wide audience. Presentations will be chosen from submitted abstracts or by invitation.

01.02 Computational Methods: Macromolecular Structure Solution and Refinement

Tom Terwilliger, terwilliger@lanl.gov

Ralf Grosse-Kunstleve, rwgk@cci.lbl.gov

This session is intended to present the latest and most exciting new developments in the area of macromolecular structure determination methods. Of special interest are methods designed to increase automation in high-throughput environments.

Presentations will be chosen from submitted abstracts or by invitation.

Speakers:

Pavel Afonine, Lawrence Berkeley Lab

Serge Cohen, NKI, Netherlands

Ethan Merritt, Univ. of Washington

Charles Weeks, Hauptman-Woodward Inst.

Min Yao, Hokkaido Univ., Japan

01.03 Large Macromolecular Assemblies

Thomas Earnest, tnearest@lbl.gov

Brian Wimberly, bwimberly@Rib-x.com

Large macromolecular complexes form much of the machinery of life. Advances in methodology are making these large complexes increasingly amenable to structure determination. This session will focus primarily on structures of large asymmetric assemblies and on methods used to determine their structures and dynamics.

Speakers:

David Bushnell, Stanford Univ.

John Miao, UCLA

01.04 Membrane Protein Structures

Susan Buchanan, skbuchan@helix.nih.gov

Pat Loll, pat.loll@drexel.edu

Membrane proteins represent an exciting frontier area of structural biology. These proteins represent a large fraction of all known proteins, and they mediate some of the most interesting and important processes known to biology, yet only recently have their structures begun to be elucidated at any appreciable rate. This session will be devoted to new structures of membrane proteins and to advances in membrane protein structure analysis. Presentations in this session will be chosen from submitted abstracts or by invitation.

01.05 Difficult Structures

Charles Carter, carter@med.unch.edu

Tina Izard, tina.izard@stjude.org

As the “low-hanging fruit” gets more thoroughly harvested, production of new macromolecular crystal structures depends increasingly on finding solutions to new problems, those typically identified with “problem” structures. The usual problems of obtaining good crystals, extracting appropriate structure factor amplitudes from noisy data, interpreting noisy maps, refining recalcitrant structures at moderate resolution, and correcting mistaken interpretations along the way all afford us with instructive experiences. In this session, we hope to assemble current examples of such problems and their solutions.

01.06 Proteins Involved in Immune System and Pathogen Interactions

Peter Sun, sun@vger.niddk.nih.gov

Edward Collins, edward_collins@med.unc.edu

As part of the Biomacromolecular Special Interest Group's desire to evolve and meet the needs of our membership, each year we will focus on a different special topic with a focus on crystallography. This year's session will focus on proteins involved in host-pathogen interactions at the cell interface. This exciting session will cover proteins that viruses and bacteria use to circumvent recognition by the host immune system. And, with a mind to giving equal time, we will also examine the host's response to viral and bacterial pathogens. Presentations will be by invitation and two abbreviated talks will be chosen from submitted abstracts.

Acknowledgement is made to Pfizer for partial support of this session.

Also see Jointly Sponsored Sessions 13.06 and 13.08.

General Interest Sessions

See Jointly Sponsored Sessions 13.10 and 13.14

Industrial SIG Sessions

04.01 Structural Biology in Industry

Paula Fitzgerald, paula_fitzgerald@merck.com

Herb Klei, herbert.klei@bms.com

This half-day session will focus on the use of X-ray crystallography to advance structural biology from an industrial perspective. It will focus on examples of structure-assisted drug design, commercial enzyme development, and small-molecule characterization. Speakers will be encouraged to emphasize how recent advances in hardware and software, particularly automation, have contributed to the success of their projects. Industrial contributions to the crystallographic community in terms of structures, software, and process development will also be presented. Attendees should leave with an understanding of what industrial crystallographers do, the tools and technologies used, and what the future might hold. Presentations will be drawn from submitted abstracts and by invitation.

Also see Jointly Sponsored Session 13.03

Materials SIG Sessions

05.01 Non-Ambient Crystallography

Olga Degtyareva, o.degtyareva@gl.ciw.edu

The focus of this session will be on high-temperature, high-pressure crystallography, used to study a wide range of material from pure elements to compounds and alloys, including minerals and the synthesis of novel materials. The session will cover recent experimental results as well as modern theoretical considerations.

Speakers:

Eugene Gregoryanz, Univ. of Edinburgh, UK

Valentina Degtyareva, Russian Academy of Sciences

Chrystele Sanloup, Univ. Pierre et Marie Curie, France

Also see Jointly Sponsored Sessions 13.01, 13.03, 13.05, 13.09, 13.12 and 13.13

Neutron Scattering SIG Sessions

See Jointly Sponsored Sessions 13.04, 13.09 and 13.15

Powder Diffraction SIG Sessions

See Jointly Sponsored Sessions 13.03, 13.04, 13.12, 13.13 and 13.15

Service Crystallography SIG Sessions

See Jointly Sponsored Sessions 13.02, 13.05 and 13.07.

Small Angle Scattering SIG Sessions

09.01 Grazing Incidence Methods for Nanoscience and Biotechnology

Jin Wang, wangj@aps.anl.gov

Randle Winans, Rewinans@anl.gov

In situ and real-time characterization of two-dimensional nanostructures and their assembly processes will be the focus of this session.

09.02 Bio-Macromolecular Assemblies

Hiro Tsuruta, tsuruta@slac.stanford.edu

Volker Urban, urbanvs@ornl.gov

In the structural genomics era, complementary diffraction techniques such as small angle X-ray and neutron scattering are expected to play an important role in studies on biological macromolecular assemblies along with cryo-electron microscopy. This session provides a comprehensive update on technological advances in non-crystalline diffraction techniques applied to structural biology as well as several exciting recent studies benefiting from the use of these techniques.

Speakers:

Dmitri Svergun, European Molecular Biology Lab, Germany

Jack Johnson, The Scripps Research Institute

William Heller, Oak Ridge National Lab

Michel Koch, European Molecular Biology Lab, Germany

Cyrus Safinya, Univ. of California, Santa Barbara

David Tiede, Argonne National Lab

09.03 Polymer Science and Technology

David Londono, J-David.Londono@usa.dupont.com

Volker Urban, urbanvs@ornl.gov

The extreme effect of processing on properties is a unique attribute of polymeric materials. Also unique is the ability of diffraction and scattering techniques to elucidate with confidence the average structure of these materials within a length scale key for the understanding of properties, from atomic dimensions to tens of microns. We will discuss topics aimed to illustrate the profound effect that diffraction and scattering techniques have on polymer science, particularly the structural effects of the processing technology that creates interesting and useful properties. This field has grown lately to include multi-detector and *in situ* studies, on surfaces, solutions and in the bulk, and is a subject of broad industrial and academic interest.

Speakers:

Alexander Boeker, Univ. of Bayreuth, Germany

Brian Landes, Dow Chemical

Deborah Massouda, DuPont

09.04 Membranes and Membrane Proteins

Roland Winter, roland.winter@uni-dortmund.de

Tim Salditt, tsaldit@gwdg.de

In this SAS session, we are going to discuss the structural and dynamical properties of lipid bilayers, model biomembranes and their interaction with peptides and proteins, essentially using small-angle scattering, reflectivity and inelastic scattering techniques, but also complementary techniques will be discussed.

Speakers:

B. Nickel, LMU, Munich, Germany

Mitsuhiro Hirai, Gunma, Japan

M. Rheinstaedter, ILL, Grenoble

H. Huang, Houston, Texas

M. Tarek, Nancy, France

Also see Jointly Sponsored Sessions 13.11 and 13.13

Small Molecules SIG Sessions

10.01 Applications of Crystal Growth and Low-Temperature Techniques

Amy Sarjeant, xray@jhu.edu

Curt Haltiwanger, CHaltiw@Cephalon.com

Serving as a continuation of and expansion on the session organized by Doug Ho and Xiaoping Wang at the ACA 2005 meeting, this session focuses on the myriad techniques that we, as crystallographers, employ in our every day research, from how we grow crystals, to how we process the data that we harvest from them. The goal of this session is to foster an exchange of ideas and methodologies, so that both tried-and-true techniques as well as new advances are shared and discussed by the community. Participants are invited to submit papers on any of the following topics: crystal growth, selection, and handling; data collection and processing strategies; structure solution and refinement techniques; and approaches for displaying, reporting, sharing and archiving of results.

10.02 Natural Products and Drugs

Xiaoping Wang, xpawang@tamu.edu

Natural products with therapeutic potential have been inspirations for drugs and drug leads. Many small-molecule drugs introduced in the last two decades can be traced to natural products. This half-day session will focus on the isolation and structure elucidation of natural products, structural relationships of natural product to bioactivity, drug discovery involving natural products and their derivatives and mimics. Presentations will be selected from submitted abstracts and by invitation.

Speaker:

Jon Clardy, Harvard Univ.

10.03 Crystal Engineering: Supramolecular Chemistry: From Assembly to Structure and Function

Christer Aakeroy, aakeroy@ksu.edu

The concept of molecular recognition has had a profound impact upon our understanding of a range of fundamental events e.g. biomolecular activity, crystallization processes, and physico-chemical signaling mechanisms. Even though molecular recognition is

typically associated with molecules in solution, such interactions are also responsible for organizing molecules in the solid state. Translating principles of molecular recognition to predictable solid-state assembly is of key importance to the development of versatile and reliable strategies for practical supramolecular synthesis and materials science. In addition, this may also facilitate the construction of new functional materials with desirable optical, magnetic, pharmacological, or catalytic properties as well as providing rational guidelines for the synthesis of small molecules with enhanced biological activity. This symposium will bring together scientist with expertise in areas that span fundamental intermolecular interactions, crystal growth, supramolecular synthesis, inorganic and organic structural chemistry, and chemical reactivity and solid-state properties. The symposium will take place over three half-day sessions (Tuesday p.m., Wednesday a.m. and p.m.) that will (loosely) follow three themes:

- Intermolecular forces, crystal growth, and polymorphism;
- Directed assembly of extended organic and hybrid architectures;
- Function and reactivity of 'engineered' materials.

In conjunction with the symposium, a poster session will highlight recent developments in supramolecular chemistry and crystal engineering, with several poster prizes to be awarded. Presentations for oral and poster sessions are solicited.

Speakers:

Joel Bernstein, Ben-Gurion Univ. of the Negev, Israel

Makoto Fujita, Univ. of Tokyo, Japan

Wais Hosseini, Univ. Louis Pasteur, France

Guy Orpen, Univ. of Bristol, UK

Matt Peterson, Transform Pharmaceuticals

Also see Jointly Sponsored Sessions 13.01, 13.02, 13.12 and 13.14

Synchrotron Radiation SIG Sessions

11.01 Radiation Damage and Macromolecular Crystallography

Ana Gonzalez, ana@slac.stanford.edu

Sean McSweeney, seanmcs@esrf.fr

Radiation damage has become a main concern in macro-

molecular crystallography. It is not only a limiting factor in the application of crystallographic techniques to microcrystals and large molecules, but the effect on data quality in conventional experiments is also becoming recognized. This session will focus on the following topics:

- Radiation chemistry: specific damage to protein atoms at room temperature or cryogenic temperatures.
- Factors that influence radiation damage: sample temperature, radiation dose, photon energy, etc.
- Data collection and software methods to mitigate or exploit the effect of radiation damage.

Also see Jointly Sponsored Sessions 13.06, 13.07, 13.08, 13.10 and 13.11

Young Scientist SIG Session

12.01 Topics of Interest to the Young Scientist

Chad A. Haynes, cah@caltech.edu

The purpose of the Young Scientist SIG session is to provide a forum to address the needs and concerns of graduate students, postdoctoral scientists, and other scientists who are transitioning through various phases of their early careers. Following on last year's success, this year's half-day session will include many interesting topics, such as "The Interworkings of the ACA", "Professional Transitioning", and "Women in Science." Topics such as academic and industrial job development/opportunity will be addressed. Any ACA member with expertise in these areas are highly encouraged to contact the session organizer to schedule a speaking opportunity.

Also see Jointly Sponsored Etter Award Session

Joint SIG Sessions

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13.01 Crystalline Materials for Storage and Containment

SM/Material

Alicia Beatty, abeatty@ra.msstate.edu

Craig Jensen, jensen@gold.chem.hawaii.edu

This session focuses on design and synthesis of materials useful for storage or containment of small molecules (gases, liquids) or ions. Crystalline material design strategies range from coordination polymer synthesis to organic hydrogen-bonded solids, and speakers having a range of synthetic approaches will be included. The session will also reflect a variety of target species for containment or storage. Presentations for oral and poster sessions are solicited.

13.02 Whole Molecule Disorder

Service/SM

Peter Mueller, pmueller@mit.edu

Whole molecule disorder is a phenomenon that exists at least theoretically. Practically, however, this phenomenon has not been described very often and, besides the fullerenes, there are few examples in the literature. In this session we will discuss what whole molecule disorder is, whether it actually occurs in everyday structures, and, if so, how to deal with it.

The session will open with two invited 40 minute talks, the first focusing on the theory of whole molecule disorder and how to distinguish it from other effects (such as wrong space group and/or unit cell, incommensurate structures, twinning, etc.), the second talk will discuss the refinement of whole molecule disorder. After a discussion and a coffee break, several shorter talks, to be selected from contributed abstracts, will follow. Contributions are invited to give examples of all kinds and variations of whole molecule disorder, including cases where apparent whole molecule disorder turned out to be something else.

Speaker:

Håkon Hope, Univ. of California, Davis

13.03 PDF Analysis of Industrially Relevant Materials

Ind/Materials /Powder

Ian Swainson, ian.swainson@nrc.gc.ca

Many industrially-relevant materials are not perfectly ordered over a long range. The focus of this session is the application of PDF and S(Q) analysis to such materials. Papers reporting studies performed directly on such materials, the linking of useful properties to states of short range order, or method developments that may prove to be useful to future applications are solicited.

Speakers:

Thomas Proffen, Los Alamos National Lab

Matt Tucker, ISIS, Rutherford Appleton Lab, UK

Bogdan Palosz, Polish Academy of Sciences, Poland

Bjørn Clausen, Los Alamos National Lab

Andrew Goodwin, Univ. of Cambridge, UK

Wojtek Dmowski, Univ. of Tennessee

13.04 Latest Advancements in Detector Technology for Synchrotron X-ray and Neutron Diffraction Instrumentation

Neutron/Powder

Jason Hodges, hodgesj@ornl.gov

This session will focus on the latest advances in detector technology and diffraction instrumentation. Fourth generation photon sources and the upcoming commissioning of the U.S. Spallation Neutron Source are expected to deliver huge increases in brightness for both photon and neutron beams. The great challenge now is to develop the detectors that significantly improve on all aspects of current technology, especially in the areas of count rate capability, spatial and time resolution.

13.05 Difficult Organics/Organometallic Structures

Service/Materials

Lee Daniels, ldaniels@RigakuMSC.com

Papers are invited for the presentation of all kinds of difficulties arising in structures of organic and organometallic materials. The

types of problems expected are not limited to these but might include enantiomer determination, very large organic molecules, crystallization of chiral molecules, difficult crystallization problems, solvent/guest inclusion, superstructure problems, modulated organic structures, light-atom identification ambiguities, and space-group difficulties.

13.06 Structural Genomics –Big and Small

SynchRad/BioMac

George DeTitta, detitta@hwi.buffalo.edu

Ashley Deacon, adeacon@slac.stanford.edu

Large-scale structural genomic centers are rapidly mapping three-dimensional structures onto the protein family universe. At the same time, many smaller lab-based projects are adopting high-throughput technologies to pursue more detailed functional characterization of specific protein families and entire biological pathways. This session will highlight the complementarity of these approaches and will stimulate ideas for future research.

13.07 Remote Data Collection

SynchRad/Service

Greg Ferrence gferren@ilstu.edu

Robert Sweet, sweet@bnl.gov

Opportunities are arising for working crystallographers to mail their specimens to central services to have diffraction data collected by experts for both small and large molecules. These services exist both at synchrotron sources and in conventional X-ray labs. We will hear examples of such facilities and of the ancillary services that make them work.

Speakers:

Annie Héroux, PXRR/NSLS

Mike Soltis, SSRL

John Huffman, Univ. of Indiana, Bloomington

Additional speakers will be recruited from submitted abstracts.

13.08 Complementary Methods to Macromolecular Crystallography

SynchRad/BioMac

Jack Johnson, jack@scripps.edu

Alexander McPherson, amcphers@uci.edu

Mechanistic biology is frequently confronted with an experimental paradox. High resolution structures are required to develop a chemical description of macromolecular interactions, but the processes themselves are dynamic and not always amenable to high resolution methods. Protein chemists and molecular biologists have been successful in generating homogeneous components and entire complex systems that are amenable to crystallization and high resolution analysis. If the dynamics of the system are small, as in the case of some enzymes and electron transfer reactions, time-resolved studies can be performed in the context of the crystal lattice using Laue diffraction. If there are dynamic features of the biological activities that are large and/or non-homogeneous, other methods must be employed for the analysis. This session focuses on the application of techniques such as electron cryo-microscopy, solution X-ray scattering, atomic force microscopy, and mass spectrometry that complement high resolution X-ray structures of proteins and protein complexes. These methods can provide characteristics of the structural biology that cannot be obtained by crystallography alone.

Speakers:

Jack Johnson, Scripps

Alexander McPherson, Univ. California, Irvine

13.09 Time-Dependent Investigations

Neutron/Materials

Xunli Wang wangxl@ornl.gov

Neutrons and X-rays advance our understanding of materials through the determination of their structures at various length scales, from atomic scale crystal structures to nano and meso scale microstructures. The construction of high power sources and the upgrading of existing instruments are bringing up tremendous improvement in experimental capabilities, most noticeably in data collection speed. As a result, it is becoming possible to investigate structural changes as a function of time while the material is going through a transition. This session will provide a forum to discuss scientific issues underlining the development of instruments for *in situ*, time-resolved measurements, with topics ranging from nanostructured materials to residual stress

development during welding. In addition, the performance of a new generation of instruments (either through new construction or upgrade) will be covered.

Speakers:

Ian Anderson, Oak Ridge National Lab
Don Brown, Los Alamos National Lab
Alan Hewat, Institut Laue Langevin, France
Linda Horton, Oak Ridge National Lab
Anke Pyzalla, Vienna Univ. of Technology, Austria

13.10 Canadian Light Source Symposium

SynchRad/General

Lynne Howell, howell@sickkids.on.ca
James Britten, xman@mcmaster.ca

The first light from the Canadian Light Source (CLS) 2.9GeV storage ring was detected in a diagnostic beamline on December 9, 2003. Beamline commissioning began in January of 2004. Initially, the CLS will focus on research in three key areas: 1) biotechnology, pharmaceuticals and medicine; 2) mining, natural resources and the environment; and 3) advanced materials, information technologies and micro systems. This session will focus on the diffraction studies being undertaken and planned for the CLS, and the design and capabilities of the supporting beamlines.

Speakers:

Brian Shilton, Univ. of Western Ontario, Canada
Natalie Strynadka, Univ. of British Columbia, Canada
Louis Delbaere, Univ. of Saskatoon, Canada
Stefan Kycia, Univ. of Guelph, Canada

13.11 Combined Techniques in Materials Science

SA/SynchRad

Paul Fenter, fenter@anl.gov
Alec Sandy, asandy@aps.anl.gov

This session will focus on the application of complementary probes, along with small angle X-ray or neutron scattering, to the investigation of nanostructure, interfaces, kinetics and dynamics in materials.

Speakers:

Alessia Cedola, Inst. for Photonics & Nanotechnologies, Italy
Bart Goderis, Catholic Univ. of Leuven, Belgium
Vivek Prabhu, National Inst. of Standards and Technology
Norm Wagner, Univ. of Delaware

13.12 Metal-Organic Hybrids – Crystal Engineering

SM/Materials/Powder

Chris Cahill, cahill@gwu.edu

This session aims to complement existing programs involving crystal engineering, yet is distinct in our efforts to highlight materials containing a significant and/or extended inorganic component. We will therefore present systems in this forum that consist of metal centered structures such as organometallic frameworks, metal-organic frameworks/coordination polymers, and inorganic/organic composite materials such as organo-clays. Some speakers have been chosen through invitation, yet additional presentations may be chosen from submitted abstracts.

Speakers:

Jing Li, Rutgers Univ.
Pingyun Feng, Univ. of California, Riverside
Przemek Dera, Carnegie Institute of Washington
Chris Cahill, George Washington Univ.
Dwight Sweigert, Brown Univ.
Seth Cohen, Univ. of California, San Diego

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13.13 Exploring Structures from the Near Neighbor to the Nanometer Scale Using Pair Distribution Function Analysis and Small Angle Scattering

Materials/Powder/SA

Thomas Proffen, tproffen@lanl.gov

Structure determination is usually based on the analysis of Bragg reflections yielding the average structure of the material. However, many materials are quite disordered or show limited long range order as in the case of nanomaterials. By analyzing the total scattering pattern, one can obtain structural information as a function of length scale from the local structure to the medium and finally long range structure. The Pair Distribution Function (PDF) technique is a more and more popular way to obtain a picture of the 'true' structure. PDFs can now be obtained covering atom-atom distances in excess of 15 nm overlapping with the lower end of the accessible length scale by Small Angle Scattering (SAS). This session will explore the two techniques and how they can be applied in combination to obtain a more complete structural picture of complex systems ranging from biology to material science.

Speakers:

Takeshi Egami, Univ. of Tennessee

Rex Hjelm, Los Alamos National Lab

Reinhard Neder, Univ. Wuerzburg, Germany

Lise Arleth, Royal Veterinary and Agricultural Univ., Denmark

Robert Papouar, Leon Brillouin Lab, France

Katharine Page, Univ. of California, Santa Barbara

13.14 Cool Structures

SM/General

Jeanette Krause, jeanette.krause@uc.edu

Allen Oliver, alol1@berkeley.edu

The Small Molecule SIG and General Interest Group are co-sponsoring a half-day general interest/interesting-chemical-crystallography-structures symposium. Authors are invited to submit abstracts for oral presentation. If you have an unusual, interesting or otherwise cool structure (or selection of structures), this is your forum to present the material to your colleagues. Any material that is of a more broad and general interest will be welcomed. In short, anything that you consider interesting crystallography is appropriate for this symposium. If you have further questions, please contact the session chairs.

13.15 X-ray and Neutron Facilities Around the Pacific Rim

Neutron/Powder

Peter Stephens, pstephens@notes.cc.sunysb.edu

The recent growth of neutron and synchrotron sources worldwide has increased the distribution of research at the cutting edge of technology in many fields, especially crystallography (broadly construed). This session will highlight science carried out at a range of facilities around the Pacific Rim, concentrating on materials science. One of the aims of this session is to tout the availability and accessibility of facilities, with the hope of growing and strengthening their user bases. There will be room in the program for contributed talks.

Transactions Symposium: The Future of Neutron Crystallography: Smaller Crystals, Larger (Macro) Molecules

Neutron/Biomac/SM

Robert Bau, bau@usc.edu

Paul Langan, langan_paul@lanl.gov

Thomas Koetzle, tkoetzle@anl.gov

Alberto Podjarny, podjarny@igbmc.u-strasbg.fr

This year's Transactions Symposium will feature a full-day program that will highlight the advances and future prospects in neutron crystallography and especially its applications to macromolecules. The program will include several overview talks that

will provide a broad introduction to the field, including a survey of the instrumentation for neutron crystallography that is available and is planned at user facilities around the world. The results of recent experiments will be presented including neutron protein structures analyzed on BIX at JAERI (Ibaraki, Japan), LADI at ILL (Grenoble, France), and PCS at LANSCE (Los Alamos, New Mexico). Speakers will offer their visions of the exciting possibilities that will be realized with the next generation of powerful neutron sources: ISIS-TII, SNS, J-PARC, and (currently in the planning stage) NxGEN and the ESS.

Speakers:

Robert Bau, Univ. of Southern California

Nobuo Niimura, Ibaraki Univ., Japan

Alberto Podjarny, IGBMC, France

Arthur Schultz, Argonne National Lab

Lee Brammer, Univ. of Sheffield, UK

Gerald Bunick, Univ. of Tennessee

A workshop on "Methods in Neutron Protein Crystallography" is planned to precede the Transactions Symposium. Together the workshop and the Transactions Symposium will provide a comprehensive introduction to those interested in using neutron protein crystallography.

Undergraduate Research Showcase

Katherine Kantardjieff, kkantardjieff@Exchange.fullerton.edu

Marilyn Olmstead, mmolmstead@ucdavis.edu

Papers are invited for either oral presentations or posters to be given by undergraduates on their crystallography research. The studies can be from any area of crystallography, but the majority of the work being presented must have been completed by the student. In addition, presentations by mentors describing the incorporation of crystallography into undergraduate curricula and research are welcome. All undergraduate participants will receive a certificate from the American Institute of Physics and a commemorative pin. The inaugural "Undergraduate Research Poster Prize" and "Undergraduate Research Presentation Prize", sponsored by the American Institute of Physics through the Society of Physics Students will be presented to undergraduate students at the ACA banquet. The winners will each receive \$200 and a banquet ticket. Posters and oral presentations will be judged by committee, during the time the student is presenting his/her research. Presentations and posters will be judged on organization and clarity, presentation, and report of the research. To be eligible for these awards, the poster or oral presentation must describe research with a significant crystallographic component, students must demonstrate a command of the science, and students must have completed the majority of the work being presented. Please indicate your wish to be considered for either of these awards with your abstract submission.