12:10 pm 05.09.06
Characterization of Amorphous High-Surface Area Magnesium Carbonate (Upsalite) Using Laboratory Diffractometer. Céleste Reiss, Olga Narygina, Marco Sommariva, Sara Frykstrand, Johan Forsgren.

**01.11.01 Standard Practices in Crystallography II: Structure Refinement and Validation**

*Session Chair: Peter Mueller*

**01.11.01.02** 9:00 am

**01.11.01.03** 9:20 am

**01.11.01.04** 9:40 am

**01.11.01.05** 10:00 am
Coffee Break

**01.11.01.06** 10:30 am
Model-building using cryo-EM and Crystallographic Maps. Thomas Terwilliger, Paul Adams, Li-Wei Hung, Pavel Afonine, Oleg Sobolev.

**01.11.01.07** 11:00 am
Strategies to Address Challenging Macromolecular Structural Projects in the Context of an Academic Service Laboratory. Diana R Tomchick.

**01.11.01.08** 11:20 am
Validation of Macromolecular Structures. Paul Adams, Pavel Afonine, Bradley Hintze, Christopher Williams, Nigel Moriarty, Oleg Sobolev, Peter Zwart, Thomas Terwilliger, Randy Read, David Richardson, Jane Richardson.

**11:50 am**
Lunch Break

**1:30 pm**
Use (and abuse) of Restraints in Structure Refinement. Peter Müller.

**1:50 pm**

**2:15 pm**
DSR - Modelling Disorder with new GUIs for ShelXle and Olex2. Daniel Kratzert.

**2:40 pm**
Patterns of Residual Electron Density that Persist in Well-Determined Crystal Structures of Iridium Compounds. Thomas Emge.

**3:00 pm**
Coffee Break

**3:30 pm**
OH...HO Clashes in Recently Published Structures. Carl Schwalbe.

**3:50 pm**
What is Needed for Proper Structure Validation and How to Interpret and Act upon Validation ALERTS. Anthony Spek.

**4:20 pm**

**01.05.02 General Interest II**

*Session Chairs: Stacey Smith and Graciela Diaz*

**01.05.02.01** 1:30 pm
NSLS-II Biomedical Beamlines for Microcrystallography, FMX, and for Highly Automated Advanced Data Collections. Jean
TUESDAY, JULY 26


1:50 pm 01.05.02.02 UGA-APS Native SAD Pilot Program at SER-CAT 22BM for General Users. Bi-Cheng Wang, John Rose, John Chrzas, Lirong Chen, Palani Kandavelu, Dayong Zhou, Unmesh Chinte, Zheng-Qing (Albert) Fu, Zhongmin Jin, James Fait, Gerd Rosenbaum, Denny Mills.

2:10 pm 01.05.02.03 Current Status of Microfocus X-ray Sources for Chemical and Biological Crystallography. Juergen Graf, Tobias Stuerzer, Holger Ott, Andreas Kleine, Joerg Wiesmann, Carsten Michaelsen.

2:30 pm 01.05.02.04 Capability and Quality Evaluation of High-Speed Detectors. Zheng-Qing (Albert) Fu, John Chrzas, John P. Rose, Bi-Cheng Wang.

2:50 pm 01.05.02.05 Computing Infrastructure, Software Optimization for High Data Rate MX, and Real Time Analysis. Herbert J. Bernstein, Kaden Badalian, Jean Jakovcic, Edwin Lazo, Sean McSweeney, Wuxian Shi, Alexei Soares, Bob Sweet.

3:10 pm Coffee Break

3:30 pm 01.05.02.06 Low-cost Home-built Imager for Protein Crystal Screening. Thayumanasamy Somasundaram, Michael Zawrotny.

3:50 pm 01.05.02.07 CCP4 Release 7.0. Charles Ballard, Andrey Lebedev.

4:10 pm 01.05.02.08 PDB2INS - An Interface to SHELXL Refinement of Macromolecules. Anna V. Luebben, Jens Luebben, George M. Sheldrick.

4:30 pm 01.05.02.09 Primordial Proteins had No Cysteines, Tryptophans, or Methionines, Started with a Valine, and Used No Codons Ending in Adenine. William Duax, Matthew Szarzanowicz, John P Scaduto, Sanjay Connare.

4:50 pm 01.05.02.10 Structural Analysis of Diverse Members of the Cyclic Amide Hydrolase Family of Toblerone Fold Enzymes. Thomas Peat.

03.07.02 Hot Structures II

Session Chairs: Governors Square 15
David Lodowski and George Lountos

Funding provided by Beryllium

1:30 pm 03.07.02.01 A Role for SETMAR in Gene Regulation: Insights from Crystal Structures of the DNA-binding Domain in Complex with DNA? Qiu-jia Chen, Millie M. Georgiadis.

1:50 pm 03.07.02.02 Crystal Structures and RNA-binding Properties of Two Hfq Homologs from Aquifex aeolicus. Kimberly Stanek, Peter Randolph, Jennifer Patterson, Cameron Mura.

2:10 pm 03.07.02.03 Structural and Biochemical Characterization of the Frequency-interacting RNA Helicase from Neurospora crassa. Yalemi Morales, Jacqueline Johnson, Sean Johnson.

2:30 pm 03.07.02.04 Recognition of a Bacterial Alarmone Through Long-Distance Association of Two Riboswitch Domains. Christopher Jones, Adrian Ferré-D’Amaré.

2:50 pm Coffee Break

3:30 pm 03.07.02.05 Apo Structures of the Adenine Riboswitch Aptamer Domain Determined Using an X-
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American Crystallographic Association, Inc.

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Vice President ................................. Amy Sarjeant
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Continuing Education .................. Kraig Wheeler
Data, Standards & Computing ......

About the ACA
The American Crystallographic Association, Inc. (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 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 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 have always been important. The benefits of membership are the same in all categories. These include: voting privileges, Reflexions, the ACA newsletter that is published 4 times per year, complimentary subscription to the Newsletter of the International Union of Crystallography, and Physics Today, a monthly publication of AIP, and reduced rates for the International Tables for X-Ray Crystallography, Structure Reports, Journal of Applied Crystallography, and Acta Crystallographica when purchased for the member’s personal use only. ACA is a member society of the American Institute of Physics (AIP) and an Regional Associate Member of the International Union of Crystallography.

Scientific Interest Group Chairs 2016
Biological Macromolecules .......... Barry Finzel
Fiber Diffraction ......................... Joseph Orgel
General Interest ......................... Graciela Diaz de Delgao
Industrial ................................. Eugene Cheung
Light Sources .............................. Allen Orville
Materials Science ...................... James Neilson
Neutron Scattering .................... William Ratcliff
Powder Diffraction ..................... Tiffany Kinniburgh
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Small Angle Scattering ............... Alex Hexemer
Small Molecules ........................... Yulia Sevryugina
Young Scientist ............................. Martin Donakowski
Canadian Division ....................... Paul Boyle

www.AmerCrystalAssn.org

The total international membership of ACA is about 1,000 with meetings held annually. There are 12 Scientific Interest Groups (SIGs) concerned with Biological Macromolecules, Fiber Diffraction, General Interest, Industrial, Light Sources, Materials Science, Neutron Scattering, Powder Diffraction, Service Crystallography, Small Angle Scattering, Small Molecules, and Young Scientists. A special division for members residing in Canada is also active. Members may join as many of these groups that are of interest them. Each SIG is responsible for organizing sessions at Annual Meetings at least every other year.

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

MARK YOUR CALENDAR

Future ACA Meetings:

2017
New Orleans, Louisiana
Friday May 26 - Tuesday May 30

2018
Toronto, Ontario, Canada
Friday July 20 - Tuesday July 24
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**Program at a Glance**

**Morning**
- WK.02: Computational Approaches to the Structural Modelling of Biological Macromolecules using SAS
- WK.03: Serial Crystallography Data Analysis with Cheetah and CrystFEL
- WK.04: Magnetic Structure Analysis by Unpolarized Neutron Diffraction Techniques (off-sites)
- WK.05: SHEXL Workshop - Part A: Sm Mol & Solid State Chemistry

**Afternoon**
- WK.01: The CSD Python API: A Foundation for Innovation
- WK.02: Computational Approaches to the Structural Modelling of Biological Macromolecules using SAS
- WK.03: Serial Crystallography Data Analysis with Cheetah and CrystFEL
- WK.04: Magnetic Structure Analysis by Unpolarized Neutron Diffraction Techniques (off-sites)
- WK.05: SHEXL Workshop - Part B: Macromolecules

**Evening**
- Student Orientation
- Opening Reception and Exhibit Show

**SIG MEETINGS**
- Industrial
- Canadian Division
- Biological Macromolecules
- General Interest
- Poster Session I
- Poster Session II
- Poster Session III
- SIG MEETINGS Joint Service & Small Molecule
- Business Meeting for all ACA Members

**Key Notes**
- **AW.01**
  - Trueblood Award & Lecture - Axel Brunger
  - Poster Preview
  - Minerals Crystallography
  - Structure-based Drug Design
  - The Next 100 Years of Powder Diffraction

- **AW.02**
  - Etter Early Career Award & Lecture - Jason Benedict
  - General Interest
  - Crystallography in Solid State Chemistry

- **AW.03**
  - Bau Award and Lecture - Benno Schoenborn
  - Engaging Undergraduates with Crystallographic Research
  - Recent Advances in Fiber Diffraction

- **AW.04**
  - Fankuchen Award and Lecture - Elspeth Garman
  - Standard Practices II: Structure Refinement & Validation
  - Radiation Damage
  - SAS and Integrative Approaches to Complex Structures

**Additional Events**
- 2016 EXHIBIT SHOW
- Plaza Exhibit Foyer
- Planning Session for 2017 Meeting in New Orleans

**Locations**
- PBD = Plaza Ballroom
- PBABC = Plaza Ballroom A,B,C
- PBEF = Plaza Ballroom E,F

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**Notes**
- GS14 = Governors Square 14
- GS15 = Governors Square 15
- GS16 = Governors Square 16
- GS17 = Governors Square 17

**Extra Details**
- Weekend: 3:00pm-10:00pm
- Saturday: 8:00am-10:00am, 10:00am-7:30pm
- Sunday: 8:00am-10:00am, 10:00am-7:30pm
- Monday: 8:00am-10:00am, 10:00am-7:30pm
- Tuesday: 8:00am-10:00am, 10:00am-7:30pm