Workshop on Advanced Crystallography
NSF’s ChemMatCARS
Sector 15, Advanced Photon Source
Argonne National Laboratory
December 14-15, 2019

Agenda

Advanced Protein Crystallization Facility (APCF) Auditorium,
Building 446, Advanced Photon Source, Argonne National Laboratory
(https://www.anl.gov/reference/argonne-campus-map)

Internet access Instructions

Friday, December 13, 2019
19:30 – 21:00 Dinner – discussion group leaders

Saturday, December 14, 2019

08:00 – 08:45 Breakfast in the APCF Auditorium
08:45 – 08:50 Welcome by Matthew Tirrell, PI of NSF’s ChemMatCARS, The University of Chicago
08:50 – 09:00 Welcome by Carlos Murillo, NSF Program Director
09:00 – 09:25 Yu-Sheng Chen, NSF’s ChemMatCARS, The University of Chicago
Overview of the new beam line design and prospect of crystallography end station
09:25 – 09:50 Simon Coles, University of Southampton, Diamond Light Source
Synchrotron chemical crystallography in the UK: Science on the dedicated I19 beamline
09:50 – 10:10 Victor Young, University of Minnesota
Crystallography software development and data management
10:10 – 10:30 Coffee Break
10:30 – 10:55 Theodore Betley, Harvard University
Resonant diffraction
10:55 – 11:20 **Shuolong Yang**, The University of Chicago  
*Combining time-resolved photoemission spectroscopy and time-resolved diffraction to access electron-phonon coupling in complex materials*

11:20 – 11:45 **Jason Benedict**, University at Buffalo  
*Structural dynamics and serial crystallography*

11:45 – 13:00 Lunch in the APCF Auditorium  
*Open discussion of current experiments*

13:00 – 13:25 **Stephan Rosenkranz**, Argonne National Laboratory  
*3D delta – pair distribution function*

13:25 – 13:50 **Simon Grabowsky**, University of Bern  
**Krzysztof Woźniak**, University of Warsaw  
*Quantum crystallography*

13:50-14:10 **David Powers**, Texas A&M University  
*Photo-crystallography*

14:10-14:30 **Przemyslaw Dera**, University of Hawai’i at Manoa  
*High-pressure crystallography*

14:30 – 14:50 **Antonino Miceli**, Argonne National Laboratory  
*Detector needs for synchrotron diffraction techniques*

14:50 – 15:40 Break and tour of NSF’s ChemMatCARS

15:40 – 17:50 **Group Discussions** — Six topics areas will be discussed. Over the two days, attendees will rotate through four topics, two assigned and two chosen during registration.

15:40 – 16:40 Rotation Session A

16:40 – 16:50 Break

16:50 – 17:50 Rotation Session B

18:00 – 20:00 Dinner (off site; Guest House restaurant closed)

**Sunday, December 15, 2019**

08:00 – 08:45 Breakfast in the APCF Auditorium

08:45 – 10:55 **Group Discussions**

08:45 – 09:45 Rotation Session C

09:45 – 09:55 Break

09:55 – 10:55 Rotation Session D

10:55 – 12:30 **Summary Presentations by Topic Discussion Leaders**

12:30 – 13:30 Lunch in the APCF Auditorium
13:30 – 14:50  Group Report Writing
14:50 – 15:00  Closing Remarks
15:00          Workshop Adjourns