

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
(<https://chemmatcars.uchicago.edu/wp-content/uploads/2019/10/Internet-Access-instruction.pdf>)

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**