



A National Science Foundation Science and Technology Center

TUESDAY, JANUARY 13, 2015

4:00 pm - 8:00 pm Registration and Check-in Ponce Hilton lobby

WEDNESDAY, JANUARY 14, 2015

7:30 am - 8:30 am Breakfast on your own at La Terraza (included in room charge)/Continued registration

8:30 am – 11:00 am BIOXFEL STC MEETING - FOR CENTER MEMBERS ONLY – GRAN SALON B
-Welcome and Introduction: Ed Lattman
-BioXFEL Education Initiative Progress From Multiple Vantages: George Phillips, Tom Grant, Nadia Zatsepin and Anthony Hutchinson
-Run 12 Collaboration and Application Planning: John Spence

11:00 am Group Photo – Outside of Gran Salon B

11:15 am - Noon BioXFEL Education & Diversity Keynote Speaker
Paul Wyn Jennings, NSF Directorate for Education & Human Resources
“Human Intellectual Capital: The Legacy of the BioXFEL STC”

2ND INTERNATIONAL BioXFEL CONFERENCE

Noon - 1:15 pm LUNCH & CONFERENCE WELCOME – GRAN SALON A
- Abbas Ourmazd, Conference Chair, UWM
- Belinda Pastrana, Faculty, University of Puerto Rico
- Ed Lattman and John Spence, Postdoctoral Discretionary Fund Award Announcement

1:30 pm – 6:10 pm INSTRUMENTATION, NANOCRYSTALLOGRAPHY & TIME-RESOLVED I - GRAN SALON B
Discussion Leaders: Petra Fromme (ASU); Edward Snell (UB)

1:30 pm – 1:55 pm Leo Chavas (CFEL)
"Possibilities for Serial Femtosecond Crystallography at Future Light Sources"

1:55 pm – 2:05 pm Discussion

2:05 pm – 2:30 pm Evgeny Saldin (DESY)
"Perspectives of Imaging of Single Protein Molecules with the Present Design of the European XFEL"

2:30 pm – 2:40 pm Discussion

2:40 pm – 3:05 pm Franz Kaertner (CFEL)
“Large-scale and Long-term Stable Timing Distribution for Free-Electron Lasers”

3:05 pm – 3:15 pm Discussion

- 3:15 pm – 3:40 pm Marius Schmidt (UWM)
“Time-resolved Nanocrystallography of Photoactive Yellow Protein”
- 3:40 pm – 3:50 pm Discussion
- 3:50 pm – 4:15 pm COFFEE BREAK – EL PASEO ATRIUM**
- 4:15 pm – 4:40 pm Uwe Weierstall (ASU)
“Serial Crystallography in Lipidic Cubic Phase”
- 4:40 pm – 4:50 pm Discussion
- 4:50 pm – 5:15 pm Brenda Hogue (ASU)
“XFEL Diffraction of Icosahedral Virus Nanocrystals for High Resolution Structure Determination”
- 5:15 pm – 5:25 pm Discussion
- 5:25 pm – 5:50 pm Belinda Pastrana (UPR)
“An Accurate and Reproducible Analysis for Protein Aggregation”
- 5:50 pm – 6:00 pm General Discussion
- 6:00 pm – 6:25 pm Richard Kirian (ASU)
“Improving Aerosol Injectors for Single-Particle Diffractive Imaging”
- 6:25 pm – 6:40 pm General Discussion
- 6:45 pm – 8:45 pm POOLSIDE RECEPTION & POSTER SESSION**
- 9:00 PM – 10:00 PM ABYS (ASSOCIATION OF BIOXFEL YOUNG SCIENTISTS) MEETING**

THURSDAY, JANUARY 15, 2015

- 7:30 am – 8:30 am Breakfast on your own at La Terraza (included in the room charge)
- 8:45 am – 12:50 pm NANOCRYSTALLOGRAPHY I – GRAN SALON B**
Discussion Leaders: Henry Chapman (CFEL); John Spence (ASU)
- 8:45 am - 9:10 am Lars Redecke (University of Hamburg & University of Lübeck)
"In vivo Protein Crystallization and X-ray Free Electron Lasers: New Strategies for Structural Biology"
- 9:10 am - 9:20 am Discussion
- 9:20 am – 9:45 am Bill Weis (Stanford)
"XFEL Data Collection and Processing Using Fewer Crystals"
- 9:45 am – 9:55 am Discussion
- 9:55 am – 10:20 am Gebhard Schertler (PSI & ETH)
“2D Crystallography and Progress towards Understanding Fundamental Protein Dynamics”



A National Science Foundation Science and Technology Center

- 10:20 am – 10:30 am Discussion
- 10:30 am – 11:00 am COFFEE BREAK – EL PASEO ATRIUM**
- 11:00 am - 11:25 am Soichi Wakatsuki (LCLS)
"LCLS Applications to Structural Biology: The Macromolecular Femtosecond Crystallography (MFX) Project in Two-color Mode for *De novo* Phasing"
- 11:25 am – 11:35 am Discussion
- 11:35 am - 12:00 pm Axel Brunger (Stanford)
"Towards XFEL Crystallography for Challenging Biological Systems"
- 12:00 pm - 12:10 pm Discussion
- 12:10 pm- 12:35 pm Brian Abbey (La Trobe University)
"Understanding the Effects of Electron Dynamics and Structural Disorder in Protein Crystallography"
- 12:35 pm – 12:50 pm General Discussion
- 1:00 pm – 2:00 pm LUNCH - GENERAL GROUP – GRAN SALON A**
- 1:00 pm – 2:30 pm LUNCH PRESENTATION FOR STUDENTS AND POSTDOCS – GRAN SALON C**
"Opportunities in Research: Industry, Academia, National Labs and Instrumentation vs. Research Labs"
Marc Messerschmidt (BioXFEL at DESY)
Elspeth Garman (Oxford)
Abbas Ourmazd (UWM)
Kenneth Trampusch (University at Buffalo)
Paul Wyn Jennings (NSF)
Moderated by George Phillips (Rice)
- 2:45 pm – 3:45 pm PRESENTATION FOR UNIVERSITY OF PUERTO RICO STUDENTS - GRAN SALON C**
"Research and Educational Opportunities with BioXFEL"
Anthony Hutchinson (BioXFEL Education and Diversity)
Chelsie Conrad (ASU)
George Calvey (Cornell)
Rahel Woldeyes (UCSF)
- 3:45 pm – 4:15 pm ASSESSMENT MEETING FOR UNIVERSITY OF PUERTO RICO STUDENTS - GRAN SALON C**
Sarah Woodruff (BioXFEL Education Advisor)
- 4:00 pm - 6:00 pm SINGLE-PARTICLE IMAGING & SOLUTION SCATTERING – GRAN SALON B**
Discussion Leader: Michael Rossmann (Purdue)
- 4:00 pm - 4:25 pm Ali Dashti (UWM)
"Frontiers in Conformational Mapping of Molecular Machines"



A National Science Foundation Science and Technology Center

- 4:25 pm - 4:35 pm Discussion
- 4:35 pm - 5:00 pm Max Hantke (Uppsala)
"Studies on Sample Heterogeneity from Thousands of Single-particle Diffraction Patterns"
- 5:00 pm - 5:10 pm General Discussion
- 5:10 pm – 5:35 pm Christoph Bostedt (LCLS)
"The LCLS Single Particle Imaging Initiative"
- 5:35 pm – 5:45 pm General Discussion
- 6:00 pm – 8:00 pm CONFERENCE DINNER – PAVILION (OPPOSITE GRAN SALONS)**

FRIDAY, JANUARY 16, 2015

- 7:30 am – 8:30 am Breakfast on your own at La Terraza (included in room charge)
- 8:00 am – 8:30 am ASSESSMENT MEETING FOR BIOXFEL GRADUATE STUDENTS – GRAN SALON C**
Sarah Woodruff (BioXFEL Education Advisor)
- 8:45 am – 12:15 pm NANOCRYSTALLOGRAPHY II – GRAN SALON B**
Discussion Leaders: Ilme Schlichting (MPI Heidelberg); Elspeth Garman (Oxford)
- 8:45 am - 9:10 am Nick Sauter (LBNL)
"XFEL Data Processing for Good and Bad Crystals"
- 9:10 am - 9:20 am Discussion
- 9:20 am – 9:45 am Joe Luft (HWI)
"An Investigation of the Formation, Frequency, and Exclusivity of Submicron Crystals Amidst Protein Crystallization Assays"
- 9:45 am – 9:55 am Discussion
- 9:55 am – 10:20 am Sang-Kil Son (CFEL)
"Phasing with Electronic Radiation Damage at High X-ray Intensity"
- 10:20 am – 10:30 am Discussion
- 10:30 am – 11:00 am COFFEE BREAK – EL PASEO ATRIUM**
- 11:00 am - 11:25 am Lorenzo Galli (University of Hamburg)
"High Intensity Phasing"
- 11:25 am - 11:40 am General Discussion
- 12:00 pm – 12:25 pm ASSESSMENT MEETING FOR BIOXFEL POSTDOCS – GRAN SALON C**
Sarah Woodruff (BioXFEL Education Advisor)
- 12:25 pm – 1:25 pm LUNCH – GENERAL GROUP – GRAN SALON A**

- 12:25 pm – 1:25 pm** **LUNCH PRESENTATION ON PROPOSAL WRITING – GRAN SALON C**
“Research Proposal Preparation 101”
Dragana Brzakovic (NSF); John Cozzens (NSF)
- 1:25 pm – 5:25 p.m.** **TIME-RESOLVED II, SPECTROSCOPY, SOLUTION SCATTERING – GRAN SALON B**
Discussion leaders: Keith Moffat (Chicago); Majed Chergui (EPFL)
- 1:25 pm – 1:50 pm Chris Kupitz (ASU)
“Time-Resolved Femtosecond Nanocrystallography of PYP/PSII”
- 1:50 pm – 2:00 pm Discussion
- 2:00 pm – 2:25 pm Junko Yano (LBNL)
“Biological X-ray Spectroscopy Combined with Crystallography at XFELs”
- 2:25 pm – 2:35 pm Discussion
- 2:35 pm – 3:00 pm Karol Nass (MPI Heildeberg)
“Radiation Damage in Serial Femtosecond Crystallography”
- 3:00 pm – 3:10 pm Discussion
- 3:10 pm – 3:25 pm** **COFFEE BREAK – EL PASEO ATRIUM**
- 3:25 pm – 3:50 pm Stefan Hau-Riege (LLNL)
“Radiation Damage Processes in Bioimaging”
- 3:50 pm – 4:00 pm Discussion
- 4:00 pm – 4:25 pm Matteo Levantino (University of Palermo)
“Myoglobin Quake-like Motion Observed with X-FEL Radiation”
- 4:25 pm – 4:35 pm Discussion
- 4:35 pm – 5:00 pm Robert Dods (University of Gothenburg)
"Time-resolved Wide Angle X-ray Scattering and Serial Femtosecond
Crystallography of Photosynthetic Reaction Centre"
- 5:00 pm – 5:20 pm General discussion
- 5:20 pm- 5:30 pm** **CONCLUDING REMARKS**