

AGENDA

MONDAY, FEBRUARY 12TH, 2018

- 3:00 PM - ONWARDS** **ARRIVAL AND HOTEL CHECK-IN** [CLICK HERE FOR MAP FROM AIRPORT](#)
MAIN LOBBY
- 3:00 PM - 5:00 PM** **WORKSHOP AND CONFERENCE REGISTRATION**
MAIN LOBBY
- 8:30 AM - 4:00 PM** **EXTERNAL ADVISORS MEETING** [CLICK HERE FOR MAP OF MEETING SPACE](#)
JACKSON
- 6:00 PM - 7:00 PM** **POSTER SESSION SETUP**
JEFFERSON

5TH BIOXFEL INTERNATIONAL CONFERENCE

TUESDAY, FEBRUARY 13TH, 2018

- 7:30 AM – 8:30 AM** **LIGHT BREAKFAST - ST. CHARLES**
- 8:35 AM – 8:45 AM** **CONFERENCE WELCOME - ST. JAMES**
Conference Co-Chairs: James Fraser (UCSF) and Richard Kirian (ASU)
- 8:45 AM – 11:55 AM** **EXPLOITING THE TIME RESOLUTION OF SFX - ST. JAMES**
Session Chairs: George Phillips (Rice) and Christopher Kupitz (UWM)
- 8:45 AM – 9:05 AM** Takehiko Tosha (RIKEN)
Time-resolved XFEL crystallography and *in crystallo* spectroscopy for probing reaction dynamics of respiratory metalloenzymes
- 9:05 AM – 9:15 AM** Discussion
- 9:15 AM – 9:35 AM** Allen Orville (Diamond Light Source)
Dynamic Structural Biology at XFELs: Complementary Tools Applied to Metalloenzymes that Make or Break O₂ Bonds
- 9:35 AM – 9:45 AM** Discussion
- 9:45 AM – 10:05 AM** Petra Fromme (ASU)
Time-resolved femtosecond crystallography studies of photosystem II and I with X-ray Free Electron Lasers
- 10:05 AM – 10:15 AM** Discussion
- 10:15 AM – 10:45 AM** **COFFEE BREAK - THE DISTRICT**
- 10:45 AM – 11:05 AM** Tatiana Domratcheva (MPI-H)
Computational-chemistry analysis of twisted and planar photochemical intermediates provides guidance for time-resolved structure determination
- 11:05 AM – 11:15 AM** Discussion

- 11:15 AM – 11:30 AM Haiguang Liu (BCSRC)
Structure and dynamics of chloride ion pumping rhodopsin
- 11:30 AM – 11:35 AM Discussion
- 11:35 AM – 11:50 AM Leonie Flueckiger (La Trobe)
Rapid mixing and injection for studying molecular dynamics in time-resolved liquid X-ray scattering experiments
- 11:50 AM – 11:55 AM Discussion
- 12:00 PM – 1:45 PM LUNCH GENERAL GROUP - ST. CHARLES**
- 12:00 PM – 1:00 PM LUNCH PRESENTATION ON BIOXFEL OPPORTUNITIES FOR UNIVERSITY OF PUERTO RICO STUDENTS - JACKSON**
- 12:00 PM – 12:45 PM LUNCH ASSESSMENT MEETING FOR BIOXFEL POSTDOCS ONLY - MAGAZINE**
- 1:00 PM – 2:15 PM ALTERNATIVE SCIENTIFIC CAREER DISCUSSION PANEL - JACKSON**
Chair: Ganesh Subramanian (ASU)
- 2:15 PM – 5:20 PM USING XFELS ON NON-CRYSTALLINE TARGETS - ST. JAMES**
Session Chair: Abbas Ourmazd (UWM) and Ghoncheh Mashayeki (UWM)
- 2:15 pm – 2:35 pm Jochen Hub (Gottingen)
Interpretation of (time-resolved) solution X-ray scattering data by explicit-solvent molecular dynamics simulation
- 2:35 pm – 2:45 pm Discussion
- 2:45 pm – 3:05 pm Michael Brown (U of Arizona)
Femtosecond X-ray scattering of membrane proteins with a free electron laser
- 3:05 pm – 3:15 pm Discussion
- 3:15 PM – 3:45 PM COFFEE BREAK - THE DISTRICT**
- 3:45 pm – 4:05 pm Carolin Seuring (CFEL)
X-ray coherent diffraction of amyloid fibrils on graphene: past, present and future
- 4:05 pm – 4:15 pm Discussion
- 4:15 pm – 4:35pm Brenda Hogue (ASU)
Virus conformational landscapes from single-particle X-ray scattering
- 4:35 pm – 4:45 pm Discussion
- 4:45 PM – 5:15 PM POSTER BLITZ - ST. JAMES**
Session Chair: Richard Kirian (ASU) and James Fraser (UCSF)
- 6:00 PM - 9:00 PM DINNER AT BARCADIA / OHM LOUNGE [CLICK HERE FOR MAP](#)**
601 Tchoupitoulas St, New Orleans, LA 70130

WEDNESDAY, FEBRUARY 14TH, 2018

8:00 AM – 8:45 AM LIGHT BREAKFAST - ST. CHARLES

8:45 AM – 11:35 AM GETTING SAMPLE TO THE BEAM - ST. JAMES

Session Chairs: Uwe Weierstall (ASU) and George Calvey (Cornell)

8:45 AM – 9:05 AM Andrea Katz (Cornell)

Mixing injector for time-resolved crystallography at X-ray free electron lasers

9:05 AM – 9:15 AM Discussion

9:15 AM – 9:35 AM Marie Gruenbein (MPI-H)

Considerations for SFX data collection at MHz XFELs

9:35 AM – 9:45 AM Discussion

9:45 AM – 10:05 AM Sarah Perry (UMass Amherst)

Graphene Microfluidics for Room Temperature Crystallography

10:05 AM – 10:15 AM Discussion

10:15 AM – 10:45 AM COFFEE BREAK - THE DISTRICT

10:45 AM – 11:05 AM Alexandra Ros (ASU)

Droplet Microfluidics for Serial Femtosecond Crystallography with XFELs

11:05 AM – 11:15 AM Discussion

11:15 am – 11:30 am Peter Berntsen (La Trobe)

Serial crystallography development in partnership with the Australian Synchrotron

11:30 am - 11:35 am Discussion

11:35 PM – 12:30 PM LUNCH GENERAL GROUP - ST. CHARLES

11:35 PM – 12:30 PM LUNCH ASSESSMENT MEETING FOR ALL WOMEN UNDERGRADS, GRADS, AND POSTDOCS - MAGAZINE

12:30 PM – 1:30 PM KEYNOTE SPEAKER: KRISTLE MCLAUGHLIN (VASSAR) - ST. JAMES

Taking a Community Centered Approach to Diversity

1:30 PM – 4:40 PM NEW APPLICATIONS IN SFX - ST. JAMES

Session Chairs: Wei Liu (ASU) and Benjamin Stauch (USC)

1:30 PM – 1:50 PM Michael Hennig (LeadXpro)

X-ray Free Electron Laser: Opportunities for drug discovery

1:50 PM – 2:00 PM Discussion

2:00 PM – 2:20 PM Andrea Markelz (UB)

Measuring Protein Intramolecular Dynamics with Terahertz Light: Functional Changes and Relevance to Biology

2:20 PM – 2:30 PM Discussion

- 2:30 PM – 2:50 PM Matthias Frank (LLNL)
Progress with solid sample supports for weakly diffracting objects
- 2:50 PM – 3:00 PM Discussion
- 3:00 PM – 3:20 PM Adrian Mancuso (EuXFEL)
Recent advances in instrumentation and methodology for XFEL structural studies from the SPB/SFX team at the European XFEL
- 3:20 PM – 3:30 PM Discussion
- 3:30 PM – 4:00 PM COFFEE BREAK - THE DISTRICT**
- 4:00 PM – 4:15 PM Matthew Coleman (LLNL)
Using XFELs to characterize nanolipoprotein particles that form HDL and LDL complexes
- 4:15 PM – 4:20 PM Discussion
- 4:20 PM – 4:35 PM Gebhard Schertler (ETH-PSI)
Exploring G coupled protein receptors and membrane protein dynamics with X-ray free electron lasers and solution NMR
- 4:35 PM – 4:40 PM Discussion
- 4:40 PM – 6:30 PM DINNER ON YOUR OWN**
- 6:30 PM – 7:00 PM MUSICAL PERFORMANCE BY BIOXFEL QUARTET**
- 7:00 PM – 9:00 PM POSTER COMPETITION - JEFFERSON**
7:00 - 8:00 EVEN POSTERS
8:00 - 9:00 ODD POSTERS

THURSDAY, FEBRUARY 15TH, 2018

- 8:00 AM – 8:45 AM LIGHT BREAKFAST - ST. CHARLES**
- 8:00 AM – 12:00 PM POSTER SESSION CLEAN UP - JEFFERSON**
**if you do not remove your poster you risk it being thrown away.*
- 8:45 AM – 12:05 PM NEW MEASUREMENT AND ANALYSIS STRATEGIES- ST. JAMES**
Session Chair: Nadia Zatsepin (ASU) and Natasha Stander (ASU)
- 8:45 AM – 9:05 AM Iris Young (LBNL)
XFEL diffraction studies of the oxygen evolving complex of photosystem II
- 9:05 AM – 9:15 AM Discussion
- 9:15 AM – 9:35 AM Henry Chapman (DESY)
Incoherent diffractive imaging for structure determination at atomic resolution
- 9:35 AM – 9:45 AM Discussion
- 9:45 AM – 10:05 AM David Case (Rutgers)
What can we learn from MD simulations of biomolecular crystals?
- 10:05 AM – 10:15 AM Discussion

10:15 AM – 10:45 AM COFFEE BREAK - THE DISTRICT

10:45 AM – 11:05 AM Helen Ginn (Diamond Light Source Ltd. - Oxford)
The slip-and-slide algorithm: a refinement protocol for detector geometry

11:05 AM – 11:15 AM Discussion

11:15 AM – 11:35 AM Doeke Hekstra (Harvard)
TBD

11:35 AM – 11:45 AM Discussion

11:45 AM – 12:00 AM Chenghua Shao (Rutgers)
XFEL structure deposition and data architecture support in PDB

12:00 AM – 12:05 AM Discussion

12:05 AM – 12:15 PM GROUP PHOTO

12:15 AM – 1:00 PM LUNCH GENERAL GROUP - ST. CHARLES

1:00 PM – 4:00 PM BIOXFEL STC MEETING - FOR CENTER MEMBERS ONLY - ST. JAMES

1:00 PM – 4:00 PM 10 min (3 powerpoint) talks on current BioXFEL collaborations.
Speakers in alphabetical order.
John Spence

2:45 PM – 3:15 PM COFFEE BREAK - THE DISTRICT