

Dynamics, Structure, and Function in Biological Systems
Scientific opportunities at ASU Compact X-ray Free Electron Laser
Biodesign Institute, Center for Applied Structural Discovery
Arizona State University, Tempe, AZ

April 6-8, 2018

Friday April 6

- 12:30 Light lunch in Biodesign Atrium, lower level
- 1:00 Welcome (Sethuraman “Panch” Panchanathan, ASU)
- 1:05 Intro to CXFEL: Updates on the design and current status (Bill Graves, ASU)
- 1:20 Experimental outline of the CXLS & CXFEL for discoveries in Biology (Petra Fromme, ASU)
- 1:40 Special modalities available with CXFEL (John Spence, ASU)

Session 1: Time resolved SFX (Chairs: Petra Fromme and Rick Kirian, ASU)

- 2:00 Marius Schmidt (UW-Milwaukee)
[Frontiers of macromolecular time resolved crystallography](#)
- 2:20 Yun-Xing Wang (NCI/NIH)
[Studying RNA conformation change in crystals using XFEL](#)
- 2:40 Emina Stojkovic (Northeastern Illinois University)
[Myxobacterial phytochromes at CXFEL](#)
- 3:00 Summary and discussions led by the session chair

3:20 CXFEL Lab tours in Biodesign C and coffee break

Session 2: Electron diffraction methods and Synergies between CXFEL and large XFELs (Chair: John Spence and Dewight Williams, ASU)

- 4:40 Tamir Gonen (UCLA)
[MicroED conception, practice and future opportunities](#)
- 5:00 Brent Nannenga (ASU)
[MicroED method development](#)
- 5:20 Mark Hunter (SLAC)
- 5:40 Summary and discussions led by the session chair

6:30 Cocktails & Dinner at University Club

Saturday April 7

- 8:30 Breakfast in Biodesign Atrium, lower level

Session 3: Large and challenging biomolecules (Chairs: Po-Lin Chiu and Hao Yan, ASU)

- 9:00 Hasan DeMirici (Stanford Pulse Institute)
[Ambient temperature structures of classical and designer antibiotics reveal novel conformations in the ribosome](#)

- 9:20 Dirksen Bussiere
[Structure-based drug design of the Eg5 Inhibitor NVP-BQS481](#)
- 9:40 Jose Martin-Garcia (ASU)
[ASU CXLS/CXFEL: Breaking Frontiers in Structure Determination and Drug Discovery Science](#)
- 10:00 Summary and discussions led by the session chair
- 10:20 *Coffee Break*

Session 4: Scattering from non-crystalline molecules and assemblies (Chair: Stuart Lindsay, ASU)

- 10:40 Michael Brown (UA)
[Femtosecond Solution X-Ray Scattering of Membrane Proteins](#)
- 11:00 Peter Schwander (UW-Milwaukee)
[From Single-Particle Ensembles to Energy Landscapes, Function and Dynamics](#)
- 11:20 Tom Grant (U Buffalo)
[Solving the phase problem in solution scattering](#)
- 11:40 Summary and discussions led by the session chair

12:00 Lunch brought in

Session 5: Membrane proteins (Chairs: Brenda Hogue and Rebekka Wachter, ASU)

- 1:00 Vadim Cherezov (USC)
[Serial Femtosecond Crystallography of GPCRs](#)
- 1:20 Wei Liu (ASU)
[GPCR-G protein complex studies by CXFEL](#)
- 1:40 Raimund Fromme (ASU)
[Challenges and limits of membrane protein structure biology in times of X-ray Free Electron Lasers](#)
- 2:00 Summary and discussions led by the session chair

Session 6: Applications of tailored x-ray time structure (Chairs: Bill Graves and Uwe Weierstall, ASU)

- 2:20 Robert Fischetti (ANL APS)
[Monochromatic and Polychromatic Serial Crystallography and the APS-U](#)
- 2:40 George Phillips (Rice U)
[Back to the future: What to do with Compact X-ray sources](#)
- 3:00 Edward Snell (U Buffalo)
[Brilliance, rate, and accessibility – Opportunities for structural biology with an XFEL in your back pocket](#)
- 3:20 Summary and discussions led by the session chair
- 3:40 *Coffee Break*
- 4:00 Nadia Zatsepin (ASU)
[Low dose serial crystallography](#)
- 4:20 Ed Lattman (U Buffalo)
[Time resolved diffuse scattering](#)
- 4:40 Summary and discussions led by the session chair

6:00 Picnic dinner at Papago Park sponsored by the Biodesign Center for Applied Structural Discovery

Sunday April 8

8:30 Breakfast in Biodesign Atrium, lower level

Session 7: X-ray spectroscopies and novel methods (Chairs: Oliver Beckstein, ASU)

9:00 Junko Yano (UC Berkeley)

[Soft X-ray spectroscopy of biological systems](#)

9:20 Armin Wagner (Diamond Light Source)

[Tender X-rays – Adding Colours to Crystallography](#)

9:40 Ganesh Subramanian (ASU)

[Monitoring Reactions by Spectroscopy: Attoseconds to seconds](#)

10:00 Summary and discussions led by the session chair

10:20 *Coffee Break*

10:40 Chufeng Li (ASU) Pink beam MX

[PINK beam Serial Crystallography at synchrotron and CXLS](#)

11:00 Alexandra Ros (ASU)

[Microfluidic Tools for XFELs](#)

11:20 Summary and discussions led by the session chair

11:40 Bag lunch and adjourn