

Pittsburgh Diffraction Conference 2019 Scientific Program

Thursday October 24th, 2019

4:00pm to 7:30pm Registration & Reception (SNS Atrium) with Opening Talk and Welcome Reception, Leighton Coates, ORNL

Friday October 25th, 2019 C156 (Biological Diffraction)

Protein Structure and Function, Chair: Leighton Coates, ORNL

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| 9.00am to 9.45am | Electrons or photons, diffraction rules them all, Fred Dyda, NIH/NIDDK |
| 9.45am to 10.10am | Structure and dynamics of aminoacrylate intermediates of tyrosine phenol-lyase, Robert Philips, University of Georgia |
| 10.10 am to 10.35am | Direct detection of protons in oxidized and reduced human manganese super oxide dismutase, Jahuan Azadmanesh, University of Nebraska |
| 10.35am to 11.00am | Collaboration Break |
| 11.00am to 11.30am | Neutron Diffraction Studies of PLP dependent Enzymes, Tim Mueser, University of Toledo |
| 11.30am to 12.00pm | Lockdown-how mutations in penicillin-binding protein 2 confer cephalosporin resistance to <i>N. gonorrhoeae</i> , Chris Davies, Medical University of South Carolina |
| 12.00pm to 12.30pm | Substrate Binding Induces Conformational Changes in a Class A β -lactamase That Prime It for Catalysis, Patricia Langan, Lentigen Technologies |
| 12.30pm to 1.30pm | Working Lunch and Poster Session |

Frontiers in Structural Biology, Chair: John Rose, University of Georgia

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| 1.30pm to 2.00pm | Cryo-neutron structure of left-handed Z-DNA d(CGCGCG), Martin Egli, Vanderbilt University |
| 2.00pm to 2.30pm | Translation inhibition in bacteria through antimicrobial peptides and hibernation factors, Raktim Roy, The Scripps Research Institute |
| 2.30pm to 3.00pm | Sulfonate/Nitro Bearing Methylmalonyl-Thioester Isosteres Applied to Methylmalonyl-CoA Decarboxylase Structure–Function Studies, Jeremy Lohman, Purdue University |
| 3.00am to 3.30pm | Collaboration Break |
| 3.30pm to 4.00pm | Structural consequences of transforming growth factor beta-1 activation from near-therapeutic X-ray doses, Timothy Stachowski, Hauptman Woodward Institute |
| 4.00pm to 4.30pm | MacCHESS after the CHESS-U upgrade, David J. Schuller, Cornell University |
| 4.30pm to 5.00pm | SER-CAT's current and future challenges in meeting the \$815M APS-upgrade, B.C Wang, University of Georgia |

Friday October 25th, 2019 Iran Thomas Auditorium (Diffraction) Parallel session two

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| 9:00am to 10:30am | Powder Diffraction, Chair: Cora Lind-Kovacs, University of Toledo |
| 9.00am to 9.30am | Systematic Determination of Magnetic structures driven by space groups in GSAS-II, Robert Von Dreele, Argonne National Lab |
| 9.30am to 10.00am | Chemistry Perspectives to Novel Quantum Materials, Weiwei Xie, Louisiana State University |
| 10.00am to 10.30am | Probing magnetic interactions in Re-based double perovskites, Corey Thompson, Purdue University |
| 10.30am to 11.00am | Collaboration Break |
| 11.00am to 12.30am | Magnetic Diffraction, Chair: Ovi Garlea, ORNL |
| 11.00am to 11.30am | Magnetic behavior and neutron diffraction of transition metal vanadate single crystals, Joseph Kolis, Clemson University |

11.30am to 12.00pm	Modulations in magnetic materials, Margarida Henriques, CAS Institute of Physics
12.00pm to 12.30pm	Structural and magnetic properties of R_2TiO_5 (R=Dy and Yb), Haidong Zhou, University of Tennessee
12.30pm to 1.30pm Working Lunch and Poster Session	
1.30pm to 3.00pm	Total Scattering, Chair: Kate Page, University of Knoxville
1.30pm to 2.00pm	Local orbital degeneracy lifting as a precursor to an orbital-selective Peierls transition, Emil Bozin, BNL
2.00pm to 2.30pm	A disordered superspace approach to understand highly structured diffuse scattering, Ella Mara Schmidt, University of Oxford
2.30pm to 3.00pm	Total scattering as a tool for quantifying local structure in iron-based superconductors, Robert J. Koch, BNL
3.00pm to 3.30pm	Collaboration Break
3.30pm to 5:00pm	Small Molecule Crystallography, Chairs: Ben Xue (University of Knoxville), Xiaoping Wang (ORNL)
3.30pm to 4.00pm	Investigating reactivity, redox distribution, and magnetism of giant spin clusters, Theodore Betley, Harvard University
4.00pm to 4.30pm	Symmetry Breaking of a dimeric Iron(ii) hydride complex, Patrick Holland, Yale University
4.30pm to 5.00pm.	Crucial Insights from crystallography into magneto-structural phase transitions in molecule-based systems, Michael Shatruk, Florida State University

All Attendees

5.00pm to 6.00pm Poster Session

6.00pm to 8.00pm Conference Banquet (SNS Cafeteria) with after dinner presentation, The history of neutron production at ORNL, Jaime Fernandez-Baca, ORNL

Saturday October 26th, 2019 Iran Thomas Auditorium (No parallel sessions)

- 9:00am to 10:30am Diffraction, Chair: Matthias Zeller, Purdue University
- 9.00am to 9.30am STS and Diffraction Instruments, Ken Herwig, ORNL
- 9.30am to 10.00am NMR-Assisted Crystallography in Tryptophan Synthase: Proton positions, stable intermediate, and Transition States, Leonard Mueller, University of California, Riverside
- 10.00am to 10.30am Total Scattering: Crystallography going local, Helen Playford, Rutherford Appleton Laboratory
- 10.30am to 11.00am Collaboration Break
- 11.00am to 12:30pm Poster Awards and Pittsburgh Diffraction Society Business Meeting
- 12.30pm to 1.30pm Working Lunch and SNS tours
- 1.30pm to 3.00 pm Hybrid Techniques, Chair C. Rawn, University of Knoxville
- 1.30pm to 2.00pm X-ray and neutron diffraction studies of negative thermal expansion materials, Cora Lind-Kovacs, University of Toledo
- 2.00pm to 2.30pm Small-Angle Neutron Scattering as a probe of nanoscale Magnetic Dynamics, Dustin Gilbert, University of Tennessee
- 2.30pm to 3.00pm Understanding reaction pathways in YMnO_3 metathesis reactions, Rebecca McAuliffe, ORNL
- 3.00 to 5.00pm Tour of the Historic Graphite Reactor at Oak Ridge National Laboratory
- End of Conference