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

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 N. gonorrhoeae, 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

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, Rakim 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

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 YMnO3 metathesis reactions, Rebecca McAuliffe, ORNL

3.00 to 5.00pm  Tour of the Historic Graphite Reactor at Oak Ridge National Laboratory

End of Conference