

*The Pittsburgh Diffraction Society*

*Established 1943*

## *The 75th Annual Pittsburgh Diffraction Conference*

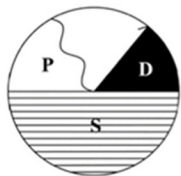
Indiana University of Pennsylvania, October 19-21, 2017

Indiana, Pennsylvania

### *Scientific Program*

The conference will feature six sessions on a wide range of topics from all fields of crystallography, such as **neutron and X-ray powder diffraction, pair distribution functions analysis, materials properties analysis and monitoring, powder diffraction of nanoparticles and metal organic frameworks, magnetic materials, and methods of structural biology**. In addition, a special Symposium will be held in memory of Bryan M. Craven and his legacy with the Pittsburgh Diffraction Society.

Preceding the PDS conference, a GSAS-II workshop will be held by **Robert Von Dreele** and **Brian Toby, ANL** on Wednesday, October 18th. This is an excellent opportunity to learn how to use this powerful software directly from the program authors. A special discount is offered for attendees of both workshop and conference.



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**Wednesday October 18<sup>th</sup>**

**GSAS-II workshop** (Chairs Robert Von Dreele, Argonne National Laboratory and Brian Toby, Advanced Photon Source, Argonne National Laboratory)

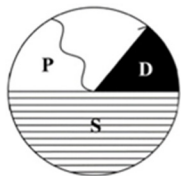
9:00 am – 10:00 pm	GSAS-II workshop
10:00 am – 10:30 am	Coffee break
10:30 am – 12:00 noon	GSAS-II workshop contd.
12:00 noon – 1:30 pm	Lunch
1:30 pm – 3:00 pm	GSAS-II workshop contd.
3:00 pm – 3:30 pm	Coffee break
3:30 am – 5:00 pm	GSAS-II workshop contd.
5:00 pm	Adjournment
7:00 pm – 8:00 pm	Opening Reception

**Thursday October 19<sup>th</sup>**

**First session:**

**Neutron powder diffraction studies of magnetic materials** (Chair Stuart Calder, HFIR, Oak Ridge National Laboratory)

9:00 am – 9:05 am	Opening Remarks
9:05 am – 9:30 am	<b>A1: Multiferroic h-LuFeO<sub>3</sub>—adventures in neutron scattering</b> <i>William Ratcliff</i> , (NCNR, NIST)
9:30 am – 10:00 am	<b>A2: Using neutron diffraction to study competing orders in unconventional superconductors</b> <i>Keith Taddei</i> (High Flux Isotope Reactor, Oak Ridge National Laboratory)
10:00 am – 10:30 am	Coffee break
10:30 am – 11:00 am	<b>A3: Powder Neutron Diffraction and Magnetic Structures of Intermetallics and Oxides: Advantages and Limitations</b> <i>John Greedan</i> (McMaster University)

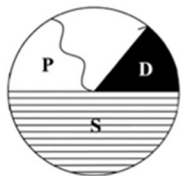


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11:00 am – 11:30 am	<b>A4: Time of flight magnetic neutron powder diffraction on POWGEN</b> <i>Simon Kimber</i> , Spallation Neutron Source, Oak Ridge National Laboratory
11:30 am – 12:00 noon	<b>A5: Spin fragmentation in Ising kagome magnets</b> <i>Martin Mourigal</i> (Georgia Tech)
12:00 noon – 1:30 pm	Lunch
<b>Second session:</b>	<b>Powder diffraction from nanoparticles</b> (Chair Cevdet Noyan, Columbia University)
1:30 pm – 1:35 pm	Opening Remarks
1:35 pm – 2:00 pm	<b>B1: Determining Crystallite Size with GSAS-II: Improving a Classical Technique</b> <i>Brian Toby</i> , Advanced Photon Source, Argonne National Laboratory
2:00 pm – 2:30 pm	<b>B2: The Analysis of Nanomaterials by Powder Diffraction</b> <i>Tim Fawcett</i> , International Center for Diffraction Data
2:30 pm – 3:00 pm	<b>B3: Correlating Local Crystalline Structure with X-Ray Powder Diffraction Spectra of Nanocrystals</b> <i>Shangmin Xiong</i> , Columbia University
3:00 pm – 3:30 pm	Coffee
3:30 pm – 4:00 pm	<b>B4: In-situ and high-resolution x-ray diffraction study of pyrite (FeS<sub>2</sub>) stoichiometry</b> <i>Rebecca D. McAuliffe</i> , University of Illinois at Urbana-Champaign
4:00 pm – 4:30 pm	<b>B5: Tunable Negative Thermal Expansion found in ReO<sub>3</sub>-type fluoride solid solutions</b> <i>Samuel James Baxter</i> , Georgia Institute of Technology,
5:00 pm	Adjournment
7:00 pm – 8:00 pm	Poster session

Friday October 20<sup>th</sup>



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**Third session:**

**Monitoring changes in materials properties through diffraction methods** (Chair Cora Lind-Kovacs, University of Toledo)

9:00 am – 9:05 am

Opening Remarks

9:05 am – 9:35 am

**C1: In-situ Structural Studies of Piezoelectric Materials**

*Michelle Dolgos, Oregon State University*

9:35 am – 10:00 am

**C2: Dynamic Disorder Activity of CH<sub>3</sub>NH<sub>3</sub> Groups in Directing the Crystal Structure of (CH<sub>3</sub>NH<sub>3</sub>)<sub>2</sub>AgInBr<sub>6</sub> Double Perovskite**

*Thao Tran, Johns Hopkins University*

10:00 am – 10:30 am

Coffee break

10:30 am – 11:00 am

**C3: In-situ powder diffraction studies of metal oxides under chemical looping conditions**

*Efrain Rodriguz, University of Maryland*

11:00 am – 11:30 am

**C4: Following in situ synthesis using neutron powder diffraction**

*Ashfia Huq, Oak Ridge National Laboratory*

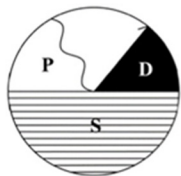
11:30 am – 12:00 noon

**C5: In situ characterization of the phase behavior and thermoelastic properties of metal oxide systems at extreme conditions**

*Leighanne Gallington, Advanced Photon Source, Argonne National Laboratory*

12:00 noon – 1:30 pm

Lunch



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**Fourth session:**

**The Applications of Emerging Methods of Structural Biology**  
(Chairs Aina Cohen, SSRL and John Rose, University of Georgia-Athens)

1:30 pm – 1:35 pm

Opening Remarks

1:35 pm – 2:00 pm

**D1: Novel Developments in Structural Biology**

*Guillermo Calero*, University of Pittsburgh

2:00 pm – 2:30 pm

**D2: *Ab initio* electron density determination directly from solution scattering data**

*Thomas Grant*, Hauptman Woodward Institute

2:30 pm – 3:00 pm

**D3: XFEL structures of the influenza M2 proton channel at 1.4 Å: room temperature water networks and insights into proton conduction**

*Jessica Thomaston*, University of California, San Francisco

3:00 pm – 3:30 pm

Coffee

3:30 pm – 4:00 pm

**D4: New Opportunities for Structural Biology Research at LCLS and SSRL**

*Aina Cohen*, Stanford Synchrotron Radiation Light Source

4:00 pm – 4:30 pm

**D5: Neutrons: Complementary Probes for Protein Crystallography**

*Leighton Coates*, Spallation Neutron Source, Oak Ridge National Laboratory

5:00 pm

Adjournment

5:30 pm – 6:30 pm

Sidhu Award Presentation and Lecture

(Chairs Ashfi Huq, Oak Ridge National Lab, Charles Lake, Indiana University of Pennsylvania, and Mary Pittman)

**S1: Sampling and Intensity Statistics of Diffraction Experiments with Nanocrystalline Powders**

*Hande Öztürk*, Brookhaven National Laboratory

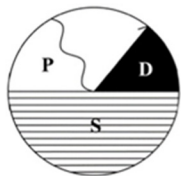
7:00 pm – 7:30 pm

Social Hour

7:30 pm

Banquet – Poster prizes

**Saturday October 21<sup>st</sup>**



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### Fifth session:

Structural analysis using atomic pair distribution functions  
(Chair Pavol Juhas, Brookhaven National Laboratory)

9:00 am – 9:05 am

Opening Remarks

9:05 am – 9:30 am

**E1: Atomic pair distribution function methods: Introduction and Applications**

*Simon J. L. Billinge*, Columbia University

9:30 am – 10:00 am

**E2: Balancing freedom and constraints in large-box PDF modeling**

*Daniel P. Shoemaker*, University of Illinois

10:00 am – 10:30 am

Coffee

10:30 am – 11:00 am

**E3: Trends in the lone pair-induced local off-centering of tin and lead atoms in halide perovskites**

*Geneva Laurita*, University of California, Santa Barbara

11:00 am – 11:30 am

**E4: Direct structural evidence of phase separation in the phase diagram of  $\text{Ir}_{1-x}\text{Rh}_x\text{Te}_2$**

*Emil S. Bozin*, Brookhaven National Laboratory

11:30 am – 12:00 noon

**E5: RMCPProfile: Moving closer to complex modelling**

*Matthew G. Tucker*, Spallation Neutron Source, Oak Ridge National Laboratory

### Special seventh session:

Symposium in memory of Bryan M. Craven (Chair John Rose, University of Georgia-Athens and Aina Cohen, SSRL)

9:00 am – 9:05 am

Opening Remarks

9:05 am – 9:35 am

**F1: In memory of Bryan Craven: My Postdoctoral Work with Him and Continuing**

*Bi-Cheng Wang*, University of Georgia

9:35 am – 10:05 am

**F2: Some personal recollections of Bryan Maxwell Craven**

*Robert Blessing*, Hauptman Woodward Institute

10:05 am – 10:30 am

Coffee

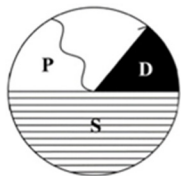
10:30 am – 11:00 am

**F3: DNA: Not Merely the Secret of Life**

*Nadrian Seeman*, New York University

11:00 am – 11:30 am

**F4: Archiving Structural Models Derived using**



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### integrative/Hybrid Methods

*Helen Berman, Rutgers University*

11:30 am – 11:50 noon **F5: Application of structural biology in biologic drug discovery**

*Jinquan Luo, Janssen R&D, LLC, Johnson & Johnson*

11:50 am – 12:10 noon **F6: Memories**

*John Ruble, University of Pittsburgh and New Century Pharmaceuticals, Huntsville AL (retired)*

12:00 noon – 1:30 pm Bryan M. Craven Lunch

**Sixth session: Powder Diffraction Studies of Metal Organic Frameworks**  
(Chair Winnie Wong-Ng, NIST)

1:30 pm – 1:35 pm Opening Remarks

1:35 pm – 2:00 pm **G1: Combined DSC-XRD for rapid simultaneous screening of phase evolution and thermal properties.**

*John B. Parise, Stony Brook University*

2:00 pm – 2:30 pm **G2: In situ Powder Diffraction Measurements of Metal Organic Frameworks at 17-BM: Modern Techniques and Methods of Structural Analysis**

*Andrey A. Yakovenko, Advanced Photon Source, Argonne National Laboratory*

2:30 pm – 3:00 pm **G3: Application of Powder Diffraction in MOF Research: Rigid and Flexible Frameworks**

*Tomče Runčevski, University of California at Berkeley*

3:00 pm – 3:30 pm Coffee

3:30 pm – 4:00 pm **G4: Neutron Powder Diffraction studies of small molecules adsorbed in MOFs**

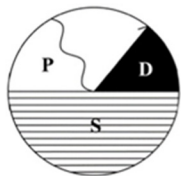
*Craig Brown, University of Delaware*

4:00 pm – 4:30 pm **G5: Linking Microstructure and Structure to Sorption Properties During Selective Gas Adsorption in Metal Organic Framework (MOF) Materials**

*Andrew J. Allen, National Institute of Standards*

5:00 pm – 5:30 pm All Members Business Meeting

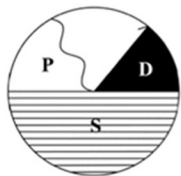
5:30 pm Adjournment



**Poster Session:**

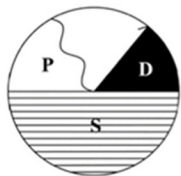
- P1: Developing metal organic frameworks for catalysis applications**  
Allison M. Rabon, Michael C. Young, Department of Chemistry and Biochemistry, The University of Toledo
- P2: Unlocking the structure of mixed amorphous-crystalline ceramic oxide thin films synthesized under low temperature electromagnetic excitation**  
Nathan Nakamura, Department of Mechanical Engineering, Carnegie Mellon University
- P3: Effect of Indium and Antimony doping on the electrical transport properties of direct vapour transport (DVT) grown SnSe single crystals**  
Shivam Patel, S. H. Chaki, and P. C. Vinodkumar, P.G. Department of Physics, Sardar Patel University, India
- P4: Reversible oxygen intercalation of  $RFe_2O_4$  (R= Lu, Yb, Y, In) as studied by in situ powder diffraction.**  
Rishvi Jayathilake, Department of Chemistry and Biochemistry, University of Maryland,
- P5: Switching Thermal Conductivity in Mn-Doped  $NiMn_xGe$**   
S. Murray, Q. Zheng, D. Cahill, D. Shoemaker, University of Illinois at Urbana-Champaign
- P6: SER-CAT Staff Research and UGA-APS Pilot Program: Extending the Concept of Visible Light Color Photography to Synchrotron Crystallography**  
Bi-Cheng Wang, John Rose, John Chrzas, Lirong Chen, Palani Kandavelu, Dayong Zhou, Unmesh Chinte, Zheng-Qing Fu, Zhongmin Jin, James Fait, Gerold Rosenbaum, and Dennis Mills, University of Georgia, Athens and Advanced Photon Source
- P7: Low temperature synthesis of molybdenum oxide for future use in composites**  
Brittany Wilson and Cora-Lind-Kovacs, Department of Chemistry and Biochemistry,





University of Toledo

- P8: *In situ* X-ray powder diffraction study on iron oxide for ammonia decomposition reaction**  
Dr. Jo-Chi Tseng, Dr. Claudio Pistidda, Dr. Claudia Weidenthaler, Deutsches Elektronen-Synchrotron (DESY), Department of Nanotechnology, Institute of Materials Research / Materials Technology, Helmholtz-Zentrum Geesthacht, Max-Planck-Institut für Kohlenforschung
- P9: Bence-Jones Protein Pav: the first ISIR structure**  
John P. Rose, Chung Soo Yoo, William Furey, Chong-Hwan Chang, Martin Sax, Bi-Cheng Wang - Work carried out in the Biocrystallography Laboratory, Veterans Administration Hospital, Pittsburgh, and the Department of Crystallography, University of Pittsburgh
- P10: Polycrystalline XRD data from a single crystal instrument with CMOS detector**  
A.Y. Nazarenko, M.S. Goodman, P. C. Ravines and A. N. Shugar, State University of New York, College at Buffalo
- P11: Synthesis and characterization of  $Al_xSc_{2-x}Mo_3O_{12}$  using non-hydrolytic sol-gel Methods**  
La'Nese Lovings, Cora Lind-Kovacs, Department of Chemistry and Biochemistry, The University of Toledo
- P12: Structure and Dynamics of Main-Group Halide Perovskite Photovoltaics**  
D. H. Fabini, E. C. Schueller, G. Laurita, C. C. Stoumpos, T.-A. Siaw, S. Han, M. G. Kanatzidis, and R. Seshadri, University of California, Santa Barbara, Bates College, Northwestern University
- P13: Synthesis and structural characterization two new  $I_4-II-IV_2-VI_7$  diamond-like semiconductors**  
Evan T. O'Hara, Stanislav S. Stoyko, Jennifer A. Aitken, Duquesne University
- P14: Synthesis and Characterization of New Diamond-like Semiconductors with Potential as Nonlinear Optimal Materials**  
Jennifer R. Glenn<sup>1</sup>; and Jennifer A. Aitken, Duquesne University
- P15: Neutron diffraction study of the temperature-dependent magnetic ordering of  $LiMn_xFe_{1-x}PO_4$**   
Stephanie Gnewuch, University of Maryland



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**P16: Metastable layered metal chalcogenides: from superconductivity to ferromagnetism**

B. Wilfong, X. Zhou, H. K. Vivanco, and E. E. Rodriguez, University of Maryland

**P17: Softchemical routes to new iron phosphates**

Prashanth Sandineni & Amitava Choudhury, Department of Chemistry, Missouri University of Science and Technology