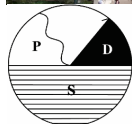


# The 76<sup>th</sup> Annual Pittsburgh Diffraction Conference Case Western Reserve University

at the Iris S. and Bert L.  
Wolstein Research Building

October 14-16<sup>th</sup>, 2018  
Cleveland, OH



## The Pittsburgh Diffraction Society

### Scientific Program

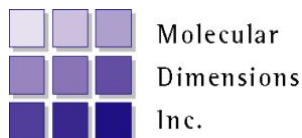
X-ray diffraction  
X-ray tomography  
X-ray free electron laser  
Cryo-electron microscopy  
Cryo-electron tomography

### Keynote Speakers

Professor Lois Pollack  
Cornell University

Professor Wah Chiu  
Stanford University

### Sponsors



## **Welcome and Introduction**

Welcome to the 76<sup>th</sup> annual Pittsburgh Diffraction Conference at Case Western Reserve University, Cleveland, OH! This conference will feature seven sessions focused on bio-macromolecules, with topics including X-ray diffraction, X-ray-tomography, X-ray free electron laser, cryo-electron microscopy, and cryo-electron tomography. We are fortunate to feature two keynote speakers: Professor Lois Pollack from Cornell University and Professor Wah Chiu from Stanford University.

We are grateful to the generous support from Case Western Reserve University School of Medicine including Departments of Physiology and Biophysics, Pharmacology, Biochemistry, Nutrition, and Pathology, as well as from our corporate sponsors TTP Labtech, Rigaku, Molecular Dimensions, MiTeGen, GE Healthcare Life Sciences, Formulatrix, FEI, Crystal Positioning Systems, Bruker, Beckman Coulter, and ARI.

The organizers Edward Yu, Tsan Sam Xiao, and Vivien Yee would like to thank the generous support from Dr. Philip Klenotic regarding abstracts; and from Denise Davis and Valerie Price at the Department of Pathology, Cynthia Ernst at the Department of Biochemistry, Kimberly Bible, Deborah Nouredine, Henry Hill, and Cathleen Hach regarding reservation and logistics. We are grateful to members of the Xiao, Yu, Yee and van den Akker labs for their tireless efforts in making this conference run smoothly. Please do not hesitate to provide comments and feedback to [ewy5@case.edu](mailto:ewy5@case.edu) and [tsx@case.edu](mailto:tsx@case.edu).

Conference Organizers: Edward Yu, Tsan Sam Xiao, & Vivien Yee

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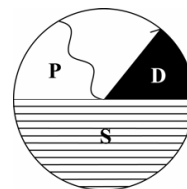
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## **The Pittsburgh Diffraction Society**

The Pittsburgh Diffraction Society (PDS) is a not-for-profit 501c3 organization which ***promotes fundamental and applied diffraction and crystallographic research and the exchange of ideas and information concerning such research.*** The society was founded by *Professor Surain S. Sidhu* who organized the first Pittsburgh Diffraction Conference (PDC) on Saturday January 16, 1943 in Lecture Room 105, Thaw Hall, University of Pittsburgh which was entitled "Conference on the Uses of X-rays, X-ray Diffraction Cameras, Electron Diffraction Cameras and Electron Microscopes." Informal remarks were given by *Surain S. Sidhu* (University of Pittsburgh), *Earl Gulbransen* (Westinghouse Research Laboratories) and *Charles S. Barrett* (Carnegie Institute of Technology), followed by discussion. The second PDC, November 3 and 4, 1944 had eleven presentations covering many diverse topics such as X-ray and electron diffraction techniques, X-ray diffraction studies of bread (no typo!), and preferred orientation in metallic systems. A banquet was held at the Webster Hall Hotel for \$2.24 pp with gratuity included. By 1947 the PDC expanded to 203 registrants including *Dorothy Crowfoot Hodgkin* (Oxford University) who presented a paper entitled "The X-ray Crystallographic Investigation of the Structure of Penicillin." In 1948, *Sir Lawrence Bragg*, Cambridge University, presented on "X-ray Structure of Proteins and Other Organic Molecules". In 1999, *Herbert A. Hauptman* presented at the annual PDC hosted by the Ohio State University. The PDC has been a continuous forum to disseminate advances in crystallography and diffraction and is currently the oldest Crystallographic society in the United States. The Pittsburgh Diffraction Society (PDS) has sponsored the annual PDC, returning to Pittsburgh, Pennsylvania area every five years. The societies founder *Professor Sidhu* is honored and remembered through the **Sidhu Award**, which is given to an outstanding scientist who is within six years of having earned a Ph.D. or its equivalent. Other awards sponsored by the PDS to support and encourage young scientists include the **George Jeffrey Award**, which provides travel assistance for students attending the triennial Congress of the International Union of Crystallography, and the **Chung Soo Yoo Award** given to the best student presenter at the annual Pittsburgh Diffraction Conference.

## Sidhu Award



The Sidhu award honors the memory of **Professor Surain S. Sidhu**, who was a Professor of Physics and Director of the X-ray Laboratory at the University of Pittsburgh. He was a founder of the Pittsburgh Diffraction Conference in 1943. Later, **Professor Sidhu** moved to Argonne National Laboratory, where he pioneered the use of the null matrix technique in neutron diffraction. This involves choosing isotopes of an element in the proportion that gives a zero net coherent scattering factor. The procedure has been widely used for studying biological materials in which the isotopic ratio of hydrogen to deuterium is appropriately adjusted. The currently biennial award recognizes an outstanding contribution to crystallographic or diffraction research by a young investigator whose doctoral degree was conferred within six years before the award date. The award carries a cash prize of \$5,000. Previous winners are:

1967 A.I. Bienenstock  
1968 R.M. Nicklow  
1969 T.O. Baldwin  
1970 S.-H. Kim  
1971 L.K. Walford  
1972 D.E. Sayers  
1974 B.C. Larson & N.C. Seeman  
1975 P. Argos  
1978 K. Hodgson & G. DeTitta  
1980 G. Petsko  
1985 D.C. Rees  
1986 D. Agard & J.M. Newsam  
1988 Q. Shen  
1989 M. Luo  
1990 L. Brammer  
1992 R.C. Stevens  
1993 M. Pressprich & T. Yeates

1994 A. Vrielink & J. Wang  
1995 M. Georgiadis  
1996 M.J. Regan  
1999 C. Ban & M. Wahl  
2000 W.R. Wikoff  
2001 L. Shapiro  
2002 Y. Lee  
2003 E. O. Saphire  
2004 Y. Xiong  
2005 C.-Y. Ruan  
2006 P. Chupas  
2008 M. Hanson  
2010 H. Wu  
2013 T.D. Grant  
2017 Hande Öztürk  
2018 Yen-Ting Lai

## **Sidhu Awardee 2018**

### **Yen-Ting Lai, Ph.D., NIH/VRC**



Dr. Yen-Ting Lai received his PhD from the University of California Los Angeles in 2013 and is currently a postdoctoral researcher at the Vaccine Research Center of the National Institute of Allergy and Infectious Diseases in Bethesda, Maryland. During his PhD, he studied protein self-assembly in Dr. Todd Yeates' lab. In this line of research, he designed and created proteins that self-assembled into tetrahedral and octahedral cages, the structures of which were verified by diverse biophysical methods including x-ray crystallography, small-angle x-ray scattering, electron microscopy and native mass spectrometry. The successful demonstration of the ability to design protein assemblies by multiple labs over the past several years has spawned wide spread interest in using artificial protein assemblies in nano-materials and nano-medicines. In his current position with Drs. Peter Kwong and John Mascola at the NIH, he engineered protein lattices to obtain high resolution structures of HIV-1 envelope glycoprotein in complex with small molecule inhibitors of the Fostemsavir class, one of which is currently in phase III clinical trials. The accurate determination of protein interactions with the diverse functional groups in the Fostemsavir derivatives allows for further improvements in drug properties and may lead to next generation HIV-1 entry inhibitors.



## Chung Soo Yoo Award



Shozo Takagi's Wedding. **Chung Soo Yoo** is on the very right.  
(Photo provided by Helen Berman)

**Dr. Chung Soo Yoo**, Adjunct Associate Professor in the Department of Medicinal Chemistry and Research Associate in the Department of Crystallography of the University of Pittsburgh, was killed in the Korean Airlines Flight 007 disaster of 31 August 1983. **Dr. Yoo** came to the U.S. from Korea in 1965; he obtained his M.S. Degree in Chemistry at Rice University in 1967 and his Ph. D. in Crystallography at the University of Pittsburgh in 1971, and became a U.S. citizen. He was a member of the Biocrystallography Laboratory of the Veterans Administration Medical Center in Pittsburgh.

**Dr. Yoo** was one of the most likeable crystallographers among students and colleagues in Pittsburgh, and was always very enthusiastic about the Pittsburgh Diffraction Conference.

The **Chung Soo Yoo Award**, established by the Pittsburgh Diffraction Society to honor **Dr. Yoo's** memory, is given to a graduate student presenting the best poster at the annual Pittsburgh Diffraction Conference and carries a cash prize of \$400.

## **The PDS Award Funds**

Over the years, the Pittsburgh Diffraction Society has created and bestowed awards to scientists and students involved in the many facets of diffraction study of matter. The first of these is the **Sidhu Award**, which recognizes the work of a young scientist who has made outstanding contributions to diffraction science within six years of earning a Ph.D. The second of these is the **Chung Soo Yoo Award**, which is given to the graduate student with the best poster presentation at a Pittsburgh Diffraction Conference. The most recent of these awards is the **George A. Jeffrey Award** given to meritorious graduate students who desire support to attend the triennial meeting of the International Union of Crystallography.

The three awards were established with generous gifts from family and friends of *Surain S. Sidhu*, *Chung Soo Yoo*, and *George Jeffrey*. We are seeking help to secure a more solid financial footing for the three PDS award funds. Please consider making a generous donation to the Pittsburgh Diffraction Society targeting one or more of the award funds.

Checks should be sent to the PDS Treasurer, **Dr. Matthias Zeller**, Purdue University, 560 Oval Drive, West Lafayette, Indiana 47907 (zeller4@purdue.edu)

*The PDS is a 501c3 organization and all donations are tax deductible in the USA; check with your tax consultant in foreign countries.*



# Pittsburgh Diffraction Conference 2018 Scientific Program

## Sunday October 14<sup>th</sup>, 2018

5:00 - 8:30 pm      Registration & Reception

## Monday October 15<sup>th</sup>, 2018

8:00 - 8:50 am      Continental Breakfast

8:50 - 9:00 am      **Opening remarks**

9:00 - 10:15 am      **Session 1: X-ray crystallography**

Moderator: Yinghua Chen, Case Western Reserve University

9:00 - 9:25 am      Edward Snell, Ph.D., Hauptman-Woodward Medical Research Institute  
*High-throughput identification and structural remediation of promiscuous metals in macromolecular structures*

9:25 - 9:50 am      Focco van den Akker, Ph.D., Case Western Reserve University  
*Crystallographic and Molecular Dynamics Approaches to Gain Mechanistic Insights into the Doughnut-Shaped Lytic Transglycosylase from Campylobacter jejuni*

9:50 - 10:15 am      Leighton Coates, Ph.D., Oak Ridge National Laboratory  
*Anomalous X-ray Diffraction Studies of Ion Transport in K<sup>+</sup> channels*

10:15 - 10:30 am      Coffee break

10:30 – 11:15 am      **Session 2: Vendor program**

Moderator: Chuck Luke, TTP Labtech Inc.

10:30 - 10:45 am      Vendor introduction

10:45 - 11:00 am      Joseph D. Ferrara, Ph.D., CSO, Rigaku Americas Corporation  
*Tools for Structural Biology from Rigaku*

11:00 - 11:15 am      Jian Xu, Ph.D., Formulatrix, Inc.  
*Formulatrix Technology: in the Frontier of Macromolecular Crystallization*

11:15 - 12:00 pm      **Sidhu Award** (Introduction by Tsan Sam Xiao, Case Western Reserve University)

**Yen-Ting Lai, Ph.D., NIH/VRC**

*Engineering of protein assemblies and crystals based on the principle of symmetry*

**12:00 – 1:00 pm**     **Keynote address** (Introduction by Edward Yu, Case Western Reserve University)

**Lois Pollack, Ph.D., Cornell University**

*Structural enzymology at X-ray free electron laser sources: Detecting angstrom-scale motions with millisecond resolution*



**1:00 pm - 2:30 pm**     **Lunch and poster session**

Poster judging by Edward Snell (Hauptman-Woodward Medical Research Institute), Sichun Yang (CWRU), and Shoucheng Du (University of Pittsburgh)

**2:30 - 3:45 pm**     **Session 3: X-ray and neutron diffraction, X-ray tomography**

Moderator: Ardeschir Vahedi-Faridi, Case Western Reserve University

2:30 - 2:55 pm     Bi-Cheng Wang, Ph.D., University of Georgia  
*SER-CAT Scientific Highlight and Facility Upgrade During APS Shutdown*

2:55 - 3:20 pm     David Lodowski, Ph.D., Case Western Reserve University  
*Probing the dynamics of GPCR allosteric activation using radiolytic footprinting*

3:20 - 3:45 pm     Shuo Qian, Ph.D., Oak Ridge National Laboratory  
*Small-Angle Neutron Scattering for Biomacromolecule Research*

3:45 - 4:00 pm     Coffee break

**4:00 - 4:50 pm**     **Session 4: X-ray free electron laser**

Moderator: Vivien Yee, Case Western Reserve University

4:00 - 4:25 pm     Aina Cohen, Ph.D., SLAC National Accelerator Laboratory  
*New Opportunities for Structural Biology Research at LCLS and SSRL.*

4:25 - 4:50 pm     Thomas J. Lane, Ph.D. SLAC National Accelerator Laboratory  
*Putting the femtosecond in SFX: ultrafast time-resolved crystallography*

**4:50 - 5:35 pm**     **PDS business meeting**

**6:30 pm**     **Banquet at Mia Bella Restaurant** (Tel: 216-795-2355)  
12200 Mayfield Road, Cleveland, OH 44106

## Tuesday October 16<sup>th</sup>, 2018

8:00 - 8:45 am Continental Breakfast

### 8:45 - 10:15 am Session 5: "The Rising Stars"

Moderator: Vijay Kumar, Case Western Reserve University

8:45 - 9:00 am John Alvarado, Ph.D., University of Pittsburgh  
*Impact of Lipid Binding Domains on the Interaction Between HIV-1 Nef and the Src-family Kinase Hck Unique-SH3-SH2 Region*

9:00 - 9:15 am Jie Yang, Case Western Reserve University  
*Mechanism of gasdermin D recognition by inflammatory caspases and their inhibition by a gasdermin D-derived peptide inhibitor*

9:15 - 9:30 am Alex Noble, Ph.D., New York Structural Biology Center  
*Tomography for Everyone: Fiducial-less Tilt-series Alignment in Appion-Protomo, Enabling CryoET of All Specimen Types*

9:30 - 9:45 am David Chmielewski, Stanford University  
*Cryo-EM structure and in-situ assembly of alphaviruses, an enveloped virus family*

9:45 - 10:00 am Chufeng Li, Ph.D., Arizona State University  
*Time-resolved X-ray free-electron laser diffraction*

10:00 - 10:15 am Jani Reddy Bolla, Ph.D., University of Oxford  
*Direct observation of the influence of cardiolipin and antibiotics on lipid II binding to MurJ*

10:15 - 10:30 am Coffee break

### 10:30 - 12:00 pm Session 6: Cryo-ET, Cryo-EM, and X-ray crystallography

Moderator: Yvonne Gicheru, Case Western Reserve University

10:30 - 10:55 am Gerry McDermott, Ph.D., UCSF/LBNL  
*Using Diffraction to Image Mesoscale Biology*

10:55 - 11:20 am Jason Mears, Ph.D., Case Western Reserve University  
*Structural Studies that Define Regulatory Interactions within the Mitochondrial Fission Machinery*

11:20 - 11:45 am Sudha Chakrapani, Ph.D., Case Western Reserve University  
*Cryo-EM reveals near-atomic details of serotonin-activation of the full-length 5-HT<sub>3A</sub> receptor*

11:45 – 12:00 pm    Wuxian Shi, Ph.D., Case Western Reserve University, BNL  
*The Micro-focusing Macromolecular Crystallography Beamlines at NSLS-II*

**12:00 – 1:00 pm    Keynote address** (Introduction by Edward Yu, Case Western Reserve University)

**Wah Chiu, Ph.D., Stanford University**

*Cryo-EM, an imaging tool beyond crystallography*



**1:00 pm - 2:30 pm    Lunch and poster session**

Poster judging by Edward Snell (Hauptman-Woodward Medical Research Institute), Sichun Yang (Case Western Reserve University), and Shoucheng Du (University of Pittsburgh)

**2:30 - 4:10 pm    Session 7: Cryo-EM and Cryo-ET**

Moderator: Elizabeth Sweeny, Lerner Research Institute, Cleveland Clinic

2:30 - 2:55 pm    Huilin Li, Ph.D., Van Andel Institute  
*Cryo-EM reveals the evolutionary path of modern-day respiratory complexes*

2:55 - 3:20 pm    Phoebe Stewart, Ph.D., Case Western Reserve University  
*Cryo-EM studies of nanoparticles*

3:20 - 3:45 pm    Derek Taylor, Ph.D., Case Western Reserve University  
*Structural characterization of the anthrax pore intermediate sheds light on the mechanism of pH-induced, membrane-spanning pore maturation*

3:45 - 4:10 pm    Xinghong Dai, Ph.D., Case Western Reserve University  
*Sub-particle cryo-EM reveals asymmetric features of the icosahedral capsid in Kaposi's sarcoma-associated herpesvirus*

**4:10 – 4:30 pm    Trainee awards and closing remarks**

## List of participants

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## Official Conference Venues

**W** Wolstein Research Building, scientific meeting (October 14-16)  
2103 Cornell Road, Cleveland, OH 44106

**C** Courtyard Marriott (Tel: 216-791-5678)  
2021 Cornell Road, Cleveland, OH 44106

**M** Mia Bella Restaurant, banquet (October 15) (Tel: 216-795-2355)  
12200 Mayfield Road, Cleveland, OH 44106  
(From Wolstein Research Building, follow Circle Drive, then right to Mayfield Rd.)

**P** Visitor Parking, **P55** and **P8**

