

American Crystallographic Association Meeting 20–24 July 2018 Toronto ON Canada

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Although dominated as usual by structural biology, there was more than enough materials crystallography to keep a powder diffractionist constantly engaged. Particularly, noteworthy were two major awards: the Warren Award to Simon Billinge, and the Buerger Award to Frank Hawthorne. In his award lecture “A series of fortunate events: How the PDF method went from niche technique to mainstream and beyond” Simon gave a history of the pair distribution function (PDF) technique, illustrated its application to a wide variety of systems, and concluded that it has a bright and exciting future. Frank’s award lecture “Bond topology and structural arrangements in inorganic crystals” discussed the application of graph theory and topology to classify and characterize several classes of layered structures (pyroxenes, amphiboles, pyriboles, and micas).

Particularly poignant were a whole-day session in honor of Dick Marsh and a lunch in honor of Judy Flippen-Anderson, a longtime mainstay of the American Crystallographic Association (ACA). The Marsh session included a number of reminiscences by crystallographers who knew and worked with Dick, as well as scientific talks. These included “Program to Find and Characterize Commensurate Modulations in Molecular Crystals” (Carol Brock), “Using Phases to Determine the Space Group” (George Sheldrick), “Out of the Marsh and into the Swamp” (Jim Kaduk), “Hypersymmetry Then and Now” (Vic Young), and “The Inverse Marsh Error” (Frank Fronczek). Kaduk’s talk considered validation of structure derived from powder data and concluded that *checkCIF* is not enough and that the crystallographer needs to actually look at the structure.

Sessions of particular interest to powder diffractionists included Neutron and X-ray Scattering on Correlated and Quantum Materials, Neutrons as Complimentary Probes for Crystals and Scattering, Materials for a Sustainable Future, New Advances in Fiber Diffraction, The Diverse World of Materials Chemistry: from Deep Space to Titanium Dioxide Nanocomposites, Crystallography at Extreme Conditions, Mineralogical Crystallography, and Operando and *in situ* Studies. Abstracts for the talks in these sessions are available on the ACA website.

A specifically “powder” session was Powder Diffraction of Industrial and Pharmaceutical Materials. This session focused on recent advances in methodology for solving crystal structures from powders and on results on industrially-relevant materials and processes. Joel Reid (Canadian Light Source) discussed the mail-in program for powder diffraction at the Canadian Light Source, using the Canadian Macromolecular Crystallography Facility (CMCF) bending magnet beamline (08B1-1 or CMCF-BM), available to industrial clients and academia. Silvina Pagola (Old Dominion University), discussed



Photo 1. (Color online) Poster session at the 2018 ACA meeting in Toronto (photo taken by Amy Gindhart).

the use of the software WinPSSP for the crystal structure determination of organic materials from powders. Elena Kabova (University of Reading, UK), discussed advances involving conformational restraints derived from crystal structures stored in the Cambridge Structural Database applied to the DASH software to solve crystal structures from powders. Jim Kaduk (North Central College, Illinois Institute of Technology, and Poly Crystallography Inc) discussed the room temperature crystal structures of large-volume pharmaceuticals solved from synchrotron data collected at 11-BM APS, followed by Amy Gindhart (International Centre for Diffraction Data, ICDD), who discussed the incorporation of room temperature powder diffraction patterns of the top 200 pharmaceutical drugs by US sales and prescription into the Powder Diffraction File databases, as part of the “Pharmaceutical Project”. Rajni Bhardwaj (Eli Lilly & Company), discussed various case studies using X-ray powder diffraction for crystal structure determination, and as a primary characterization tool during pharmaceutical solid form discovery and drug development. Luzia Germann (Max Planck Gesellschaft) talked about the use of in-situ



Photo 2. (Color online) Scene of the Banquet at the 2018 ACA meeting in Toronto (photo taken by Amy Gindhart).

monitoring methods to study the mechanisms and sequential mechanochemical formation of pharmaceutical co-crystals. Peter Stephens (Stony Brook University) discussed the crystal structure of iron(III) (deuteroporphyrin-IX), a material of interest toward the design of antimalarial drugs.

In addition to oral presentations, there were also poster sessions (Photo 1) where scientific interactions and

collaborations took place. The annual exhibit by various equipment manufacturers and publishers to demonstrate their latest products and services was a popular area that attendees often gathered around. During the meeting banquet (Photo 2), in addition to the traditional dinner speeches, a number of awards were also presented. All in all, the meeting was a great success.