THE ADVANCED PHOTON SOURCE
TOBY AND VON DREELE OF THE APS RECEIVE THE 2019 ACA TRUEBLOOD AWARD

Brian H. Toby and Robert Von Dreele of the U.S. Department of Energy's Advanced Photon Source (APS) at Argonne National Laboratory have been selected as the recipients of the American Crystallographic Association (ACA) 2019 Trueblood Award in recognition for their "seminal contribution to the crystallographic community, in the creation and support of widely-used open-source software (GSAS-II, GSAS, and EXPGUI), in development of new instrumentation, new diffraction techniques, and in training."

GSAS-II is a unique and comprehensive open source Python project diffraction-based materials characterization and crystallography for solids on all scales, from perovskites through proteins, using both powder and single-crystal diffraction and with both x-ray and neutron probes with data from laboratory and synchrotron x-rays as well as constant wavelength or time-of-flight neutron sources. It provides structure solution and refinement as well as extensive visualization capabilities.

Many capabilities of GSAS-II that are unique are only found in software with very limited scope. For magnetic scattering, all possible color subgroups can be derived and explored. With powder diffraction, GSAS-II supports all stages of data reduction and analysis, including area detector calibration and integration, pattern indexing, LeBail and Pawley intensity extraction and peak fitting. Pair distribution functions can be computed from high-energy x-ray diffraction. Instrumental profile parameters can be fit to data from standards or derived from fundamental parameters; sample profile effects (crystallite size and microstrain) are treated independently

Left: Brian Toby. Right: Robert Von Dreele

from the instrument. When large numbers of patterns are measured with changes in measurement settings, GSAS-II provides a novel capability to fit all patterns in a single sequential refinement with subsequent parametric fitting. GSAS-II also provides small-angle scattering and reflectometry fitting and the simulation of the effects of stacking faults. GSAS-II is made freely available.

Bob Von Dreele started using Rietveld analysis in the early 1970s and wrote the first TOF-neutron Rietveld code. In the 1980s, with Allen Larson, he wrote GSAS (General Structure Analysis System) for all types of crystallography, which was the first program to work with all types of experiments (single-crystal and powder, lab and synchrotron x-rays, TOF and CW neutrons). Brian Toby then added EXPGUI as a graphical front end to GSAS. However, unlike GSAS-II, GSAS/EXPGUI could only be used for structure refinement.

About 10 years ago, an Argonne workshop explored future needs for software needs in crystallography and a few years after that Bob and Brian teamed to begin coding for a next

generation replacement for GSAS and EXPGUI. That became GSAS-II, which was made available in 2013, while significant capabilities were still being added; only in the last year has it had all of the capabilities of GSAS/EXPGUI.

GSAS-II has been developed in a manner different than traditional software projects. Usually, software and documentation are created to satisfy a set of goals and are then distributed. An agile development strategy instead has been used for GSAS-II, where initially software with very limited capabilities was released. Many new features and capabilities have been added to the software since its introduction, optimizing speed, ease of use or generalizing capabilities over much of the current decade. Feedback from users has provided a valuable contribution to this process. Citations to GSAS-II have been doubling each year since 2013, with 104 citations in 2017.

Toby and Von Dreele will accept the award at the next ACA Annual Meeting in July of 2019, where they will deliver the Trueblood Award lecture and receive the awards.

For more information, see the GSAS-II home page at: http://bitly/GSASII
and
B.H. Toby and R.B. Von Dreele, "GSAS-II: the genesis of a modern open-source all purpose crystallography software package," J. Appl. Cryst. **46**(2), 544 (2013).

CALL FOR APS GENERAL-USER PROPOSALS

The Advanced Photon Source is open to experimenters who can benefit from the facility's high-brightness hard x-ray beams.
General-user proposals for beam time during Run 2019-2 are due by Friday, March 1, 2019.
Information on access to beam time at the APS is at http://www.aps.anl.gov/Users/apply_for_beamtime.html or contact Dr. Dennis Mills, DMM@aps.anl.gov, 630/252-5680.

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Advanced Photon Source
Bldg. 401/Rm A4113
Argonne National Laboratory
9700 S. Cass Ave.
Argonne, IL 60439 USA
aps.anl.gov
apsinfo@aps.anl.gov

U.S. DEPARTMENT OF
ENERGY
Office of Science
science.energy.gov/

Argonne
NATIONAL LABORATORY
anl.gov