

DIFFRAC^{plus} TOPAS

Spotlight Series Software Training



Course Description:

This course applies to users who are familiar with using an X-ray diffractometer and puts the spotlight on TOPAS.

Participants should have basic knowledge of powder X-ray diffraction. This course applies to diffractometer users who are already familiar with TOPAS software and profile fitting techniques, but want more in-depth training. To get the most out of this course, please bring datasets from your instrument for hands-on practice and one-on-one assistance. Attendees will have a computer with TOPAS software installed available for hands-on participation. (Their own or one will be provided.)

Recommended Prerequisite:

- 4-day XRD New System Applications Training class in Madison, WI or
- 2-day XRD On-site Training

Course Instructors:

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Course Outline & Agenda:

Day 1

9 am – 5 pm

- Introduction to TOPAS software
- Sample Preparation - Tips and Tricks
- Peak Profile Fitting
- Reitveld Refinement Basics and Quantitative
- Ab-initio Structure Determination: Indexing

Day 2

9 am – 5 pm

- Analysis and Hands-on: Quantitative Analysis
- Ab-initio Structure Determination: Charge Flipping
- Ab-initio Structure Determination & Simulated Annealing
- Individual training with exercises at the computer