# TOPAS Intensive Course

**June 21 - 23, 2026 – Crans Montana, Switzerland**
**Regent Congress Centre, Rte des Mélèzes 28, 3963 Crans-Montana**

# Program:

## SUNDAY, 21.06.: TOPAS BASICS and NEWS

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| 12:00 – 13:00 | **Registration** |
| 13:00 – 13:15 | Welcome<br>*Arnt Kern, Bruker AXS, DE* |
| 13:15 – 14:00 | TOPAS V8<br>*Alan Coelho, Coelho Software, AU* |
| 14:00 – 17:30 | **Theory and Exercises: Basic functions in TOPAS**<br>*Robert Dinnebier, MPI Stuttgart, DE* |
| 17:30 – 18:00 | TOPAS-Editor Tips and Tricks - Power Editing for Launch Mode<br>*John Evans, University of Durham, UK* |
| 18:00 – 18:30 | Handling lots of data<br>*John Evans, University of Durham, UK* |

Coffee will be served during exercises

## MONDAY, 22.06.: (MICRO)STRUCTURE DETERMINATION AND REFINEMENT

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| 08:30 – 11:30 | **Theory and Exercises: Whole Powder Pattern Modeling (WPPM)**<br>*Paolo Scardi, Uni Trento, IT* |
| 11:30 – 12:00 | New macros for peak profile modeling and diffuse scattering<br>*Marcelo Malagutti & Paolo Scardi, Uni Trento, IT* |
| 12:00 – 13:00 | **Lunch break** |
| 13:00 – 17:30 | **Theory and Exercises: Indexing, ab-initio structure determination and refinement**<br>*Sebastian Bette, MPI Stuttgart, DE* |
| 17:30 – 18:00 | Symmetry-dependent directional equivalences for diffraction studies<br>*Tudor Muntean[1)] & Peter Khalifah[2)],*<br>*[1)] Stony Brook University, US, [2)] Brookhaven National Laboratories, US* |
| 18:00 – 18:30 | Understanding shear defects in oxides<br>*Scott Misture, Alfred University, USA* |

Coffee will be served during exercises.

## TUESDAY, 23.06.: PAIR-DISTRIBUTION FUNCTION ANALYSIS

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| 08:30 – 12:00 | **Theory and Exercises: PDF analysis**<br>*Maxwell Terban, Momentum Transfer, DE* |
| 12:00 – 13:00 | **Lunch break** |
| 13:00 – 13:20 | hkl-based calculation of total scattering patterns from discrete and low-dimensional structure models using TOPAS<br>*Karsten Mesecke, Monash University, AU* |
| 13:20 – 13:40 | Understanding heterogeneous transformations in Li-S batteries through operando diffraction mapping<br>*Peter Khalifah, Brookhaven National Laboratories, US* |
| 13:40 – 14:00 | Synthesis and characterization of novel Ni-Mg-coordination polymers within the framework of a high school research project<br>*Sebastian Bette, MPI Stuttgart, DE* |
| 14:00 – 14:20 | Using TOPAS to study the fast and high-temperature formation of rare-earth-free magnets<br>*Jesper Simonsen. Aarhus University, DK* |
| 14:20 – … | **Wrap-Up** |