



## Workshop Title: TOPAS School

**Day1-** 2022-11-03 (Thursday), 09:00 – 18:00

**Day2-** 2022-11-04 (Friday), 09:00 – 12:30

**Place:** Ara Hall (AH)

**Registration fee:** Free (including Coffee Break)

## Workshop Synopsis

We are pleased to announce a TOPAS School with hands-on training. The primary topic of this school course is to teach participants the operation of TOPAS for structure determination and refinement from diffraction data. The school is open to all applicants interested in the structure analysis capabilities of TOPAS.

### What you will learn:

- Indexing using the LSI and LP-Search methods
- Ab-initio structure determination using Global Rietveld refinement (Simulated Annealing) and Charge Flipping methods
- Structure refinement using the Rietveld and Two-Step methods
- Use of
  - Single crystal and powder data
  - Laboratory and synchrotron Xray data, CW and TOF neutron data

### What you will do:

- Use your own laptop to determine and refine several organic and inorganic structures

**Note:** You need to bring your own, contemporary laptop to perform exercises in the hands-on sessions. You must have Win10 (32 or 64bit) installed plus administrator rights as well as functioning WLAN and USB ports. TOPAS V6 and temporary licenses will be made available onsite. If you do not want to bring a laptop or if your laptop does not fulfill the requirements, you may follow the exercises on the main screen.

## Instructor

Dr. Arnt Kern, Head of Product Management XRD  
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