TOPAS for small box Pair Distribution Function refinements

Content

TOPAS is a fast and flexible program for non-linear least squares refinement with a focus on crystallographic analysis of diffraction data. Alongside powder and single crystal diffraction data, TOPAS also allows the refinement of pair distribution function (PDF) data. Helpful tools like restraints, constraints, and rigid bodies can be used within PDF refinements to model local structure of disordered materials.

In this tutorial you will be introduced to TOPAS and its use for PDF data. Participants will be able to select from a range of tutorials to match their level and areas of interest, including:

- Modelling instrumental and processing impacts on the PDF
- Comparing ways of modelling thermal motion effects
- Modelling of nanoparticles
- Joint powder diffraction and PDF refinements
- Modelling of small molecules
- Modelling short- and long-range effects in the same model

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Contribution Type: Invited

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