

TUT 5: Hands-On Tutorial: Magnetic Structure Determination Using Fullprof and SARAh Representation Analysis (joint session MA/TUT)

The functionalities of many materials of contemporary interest are related to complex types of magnetic ordering. Accurate magnetic structure determination is thus crucial for understanding and optimizing such materials.

After an introduction into the subject, participants of the tutorial will gain hands-on experience on the methods for magnetic structure determination.

Time: Sunday 16:00–18:15

Location: TRE/PHYS

Invited Talk

TUT 5.1 Sun 16:00 TRE/PHYS

Recent advances and challenges in magnetic structure determination — ●DMYTRO INOSOV — Institut für Festkörper- und Materialphysik, TU Dresden, Germany

In this introductory tutorial talk, I will provide an overview of magnetic structure determination in the context of recent advances in magnetic materials. I will focus on the limitations and challenges of magnetic structure refinement, and explain why it is important to use the full range of complementary experimental methods alongside conventional diffraction in order to develop a consistent understanding of magnetic structures. This is particularly important when dealing with complex types of magnetic order, such as noncollinear and multi-Q spin textures, altermagnets, and systems with multiple magnetic sublattices or very weak and/or fluctuating magnetic moments.

Tutorial

TUT 5.2 Sun 16:30 TRE/PHYS

Hands-On Tutorial: Magnetic Structure Determination Using Fullprof and SARAh Representation Analysis — ●MATTHIAS FRONTZEK — Oak Ridge National Laboratory, Neutron Scattering Division, One Bethel Valley Road, 37831 Oak Ridge, TN,

USA

The determination of magnetic structures is a crucial aspect of materials science, particularly for understanding the magnetic properties of novel materials. Given the limited availability of neutrons with the closure of smaller sources, competitive access to beam time, and the high hurdles associated with software usage, there is an increasing need for training in the analysis of magnetic structures. This tutorial aims to provide participants with practical skills in magnetic structure determination using SARAh and Fullprof, two powerful tools frequently utilized in this field.

Participants will:

- Gain hands-on experience with the tools and techniques necessary for magnetic structure determination.

- Refine nuclear and magnetic structures using real data sets.

- Understand key concepts in diffraction techniques and steps involved in the magnetic structure determination process.

Important: for Hands-on participation, please bring a laptop with a working installation of Fullprof (<https://www.ill.eu/sites/fullprof/>).

For links to Fullprof, SARAh stand-alone and tutorial data visit: <https://neutrons.ornl.gov/wand/users>