



Department of Physics

Siddaganga Institute of Technology

An Autonomous Institute, Affiliated to VTU Belagavi, Approved
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B H Road, Tumakuru – 572103, INDIA



“Online-International Workshop on X-ray Diffraction Analysis”

Conducted Online (WebEx platform), during 16th to 20th October 2020

Chief Patrons

Dr. M. N. Channabasappa

Director

Dr. Shivakumaraiah

Chief Executive Officer

Patron

Dr. K. P. Shivananda

Principal

About the workshop: X-ray diffraction is the preliminary characterization technique used in the materials characterization. Phase purity, crystallinity, crystal structure, phase quantification are some of the many useful information one can derive from XRD analysis. In this virtual workshop, the participants had hands on experience on phase analysis, **Rietveld refinement**, micro-strain analysis using open source software such as **FullPROF suite** and **QualX**.

Program in brief: **On Day 1** started with the Introduction to X-ray diffraction (XRD) - basics of diffraction, Crystal structure and data acquisition technique were explained. Followed by this a brief introduction to FullPROF suite programs was provided i.e., demo on usage of WinPlotr, EdPcr, Vesta programs. **On Day 2** the participants learned the Phase Identification (PI) - to perform search match using QualX and obtain the phase information of the sample. Profile fitting using the preliminary information obtained from the PI to get the lattice parameter, space group, crystallite size, strain for the sample of interest was taught. **On Day 3** the participants are introduced to the Rietveld refinement. Demo for indexing of the unknown sample using DICVOL, TREOR, and other algorithms will be given. **On Day 4** Rietveld Refinement on single phase using the information from PI, plotting the resultant crystal structure and obtaining bond distance - angles. Further the participant's learned the procedure for quantification of the phases through Rietveld refinement on a multiphase sample in order to obtain the weight percent distribution of each phase.

Seventy Eight participants from different parts of the country and 25 participants from abroad have registered and attended the workshop. The participants had to take quizzes and assignments based on the concept of the workshop for their self evaluation. E-Certificates are issued to the participants who have attended all the sessions of the workshop and participated actively. The recorded session of the workshop can be found in the following playlist on YouTube.

<https://www.youtube.com/playlist?list=PLlgwaeedHey64dWGsWdnnVjD8VttV66ud>

Dr. Suresh Kumar H. M.

Head of Department of Physics, Co-Patron

Dr. Madhu Chennabasappa

Convener and Resource Person