





## Goa University Crystallography Workshop 2023 - GUCW-I

# ICDD® Workshop on Materials Characterization Using Powder X-ray Diffraction

Hosted by School of Chemical Sciences, Goa University in collaboration with Vivertana Distributors Pvt. Ltd.

Date: December 7<sup>th</sup> to 8<sup>th</sup>, 2023

Venue: School of Chemical Sciences Auditorium,

Science Block E, Goa University, Goa

The structure of the workshop is intended to be very interactive with lectures followed by (or along with) hands-on sessions. Hands-on sessions are designed to learn the concepts by solving problems of different complexity levels (simple to advanced)

This workshop will describe both data mining using the ICDD PDF-5+® database and methods of analysis embodied in ICDD PDF-5+® Sieve+ and ICDD MDI JADEPro® software.

Hands-on access to PDF-5+® and JADEPro® will be available through a remote desktop server via web access. Attendees should bring their laptop computer with wireless web access (Edge, Chrome, Firefox).

Note: Mac laptop (macOS) users should have Windows emulator installed

The first day of the workshop will present the PDF databases, database overview, features, datamining capabilities and Sieve+ for phase identification.

The second day will be qualitative and quantitative XRD analyses using MDI JADEPro software. In addition, materials characterization using the JADEPro Toolkit features will be demonstrated.

Attendees will have two-week (December 15th to 30th, 2023) post meeting access to PDF-5+® and JADEPro®.

#### **Speakers:**

Dr. Soorya N. Kabekkodu, Editor-in-Chief, International Centre for Diffraction Data (ICDD), USA

Professor Tayur N. Guru Row, Emeritus Professor, SSCU, Indian Institute of Science, Bangalore

Professor Arun M. Umarji, Emeritus Professor, MRC, Indian Institute of Science, Bangalore

Convener: Dean,SCS:

Dr. Digamber G. Porob Prof. Vidhyadatta M. Shet Verenkar

**Co-Conveners:** 

Dr. Savita A. Kundaikar and Dr. Kiran T. Dhavskar

Members:

Dr. Rupesh E. Patre, Dr. Hari K. Kadam and Dr. Prajesh S. Volvoikar

Registration link: https://forms.gle/5vTiqfVgHo8KgCL86

Email:

gucw@unigoa.ac.in

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Venue: School of Chemical Sciences Auditorium, Science Block E, Goa University, Goa 7<sup>th</sup> and 8<sup>th</sup>, December 2023

# **Programme Schedule**

Day 1: 7 <sup>th</sup> December 2023 (9	9:30 am to 5:30 pm)
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9:30 - 10:00am	Inaugural function
10:00 - 10:30am	High Tea
10:30 - 11:00am	Powder X-ray Diffraction Method and Applications (TNG)
11:00 – 12:30pm	Diffraction Geometry, Systematic Angular errors and calibration procedures, sample preparation (SNK)
12:30 - 1:00pm	Setting up PDF-5+ and JADEPro access
1:00 - 2:00pm	Lunch Break
2:00 – 3:30pm	Hands-on sessions: Introduction to Search/Match Procedure with PDF-5+/Sieve+, PDF-5+ Database and features overview, Data mining (SNK)
3:30 - 4:00pm	Tea Break
4:00 – 5:30pm	Phase identification methods (SNK) Qualitative and semi-quantitative (RIR) phase analysis, Advanced phase identification (with amorphous components, Trace phases), Additional problem solving, Q&A

## Day 2: 8<sup>th</sup> December 2023 (9:30 am to 5:30 pm)

9:30 - 10:00am	Data collection strategies for materials characterization (AMU)
10:00 - 11:00am	Introduction to PXRD indexing (SNK)
11:00 - 11:30am	Tea Break
11:30 – 1:00pm	Introduction to profile functions, fitting, and Quantitative Phase Analysis (QPA) using Rietveld method (SNK)
1:00 to 2:00pm	Lunch Break
2:00 to 3:30pm	JADEPro hands-on sessions (SNK) JADEPro features overview, Angular Calibration (Instrument Profile Curve, IPC) Pattern Indexing using JADE
3:30 to 4:00pm	Tea Break
4:00 to 5:00pm	JADEPro hands-on sessions (SNK) Whole pattern fitting (WPF) and Rietveld refinement, Phase identification and Quantitative Phase Analysis (Rietveld), Crystallinity measurement, Crystallite Size and Micro-Strain Analysis
5:00 to 5:30pm	Q&A, concluding remarks and feedback from participants

#### **Speakers:**

SNK – Dr. Soorya N. Kabekkodu, Editor-in-Chief, International Centre for Diffraction Data, USA TNG – Prof. Tayur N. Guru Row, Emeritus Professor, SSCU, Indian Institute of Science, Bangalore AMU – Prof. Arun M. Umarji, Emeritus Professor, MRC, Indian Institute of Science, Bangalore

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# **Workshop Information**

Online application to Register for the workshop will be available from 16<sup>th</sup> till 30<sup>th</sup> October 2023. After the application is submitted, the first 50 applicant will be shortlisted for registration and details for the payment of fees will be communicated. Selection will be based on first come first basis. Maximum number of participants (with access to software) is 50.

Participants must carry their own laptops which will be required for hands on training on crystallography software's. Mac laptop (macOS) users should have Windows emulator installed.

## **Important Dates:**

16<sup>th</sup> October 2023 - Online application to Register for the workshop will be available

30<sup>th</sup> October 2023 – Last day to submit the application

3<sup>rd</sup> November 2023 – Selected participant will be informed to pay the fees

8<sup>th</sup> November 2023 – Last day to make payment.

10<sup>th</sup> November 2023 – Confirmation of Registration

7<sup>th</sup> and 8<sup>th</sup> December 2023 – Workshop

## Registration fees:

The registration is free for all the research students and teachers of School of Chemical Sciences, Goa University.

- (i) Rs. 500/- for the research students of other Schools of Goa University and affiliated colleges.
- (ii) Rs. 1000/- for the teachers of other Schools of Goa University and affiliated colleges.
- (iii) Rs. 1000/- for the research students of all other institutes not affiliated to Goa University.
- (iv) Rs. 2000/- for the teachers of all other institutes not affiliated to Goa University.
- (v) Rs. 5000/- for participants from Industry.

Email id: gucw@unigoa.ac.in

Registration link: https://forms.gle/5vTiqfVgHo8KgCL86

#### Note:

- Refreshments and lunch will be provided on both the days.
- Outstation participants will have to make their own arrangements for accommodation and travel.
- Participants must strictly adhere to the workshop timings.
- Attendance for all sessions is mandatory to receive the certificate of participation.





