



GOA UNIVERSITY

SCHOOL OF CHEMICAL SCIENCES

Goa University Crystallography Workshop – 2024

23rd & 24th October 2024

Report

1. Title of the Event/Activity/ program	Goa University Crystallography Workshop - 2024
2. Date and Time	23rd & 24th October 2024 (Full day)
3. Mode of conduct (Physical/Online)	Physical (offline) mode
4. School/ Directorate/ Section	School of Chemical Sciences
5. Collaborating Agency/School/Directorate	Majorly funded by DST-PURSE
6. Detail of the Resource Person (Brief biodata)	Dr. Tapas Kumar Mandal; Associate Professor, IIT Roorkee Dr. Diptikanta Swain; Scientific Officer, ICT-IOC Bhubaneswar Dr. Digamber Porob; Associate Professor, Goa University Dr. Elaine T. Dias; Assistant Professor, Goa University
7. Number of Faculty attended/participated	35
8. Number of Student attended / participated	172
9. No. of external students/faculty/other participants	67
10. The objectives of the Program/activity /event	To provide in-depth knowledge and hands-on training on powder X-ray diffraction techniques

11. Description of the Program /activity/ event	Common crystallographic softwares like WinPLOTTR and Fullprof were used for hands-on training in indexing, whole powder pattern fitting, and Rietveld refinement. Multi-phase Rietveld refinement and magnetic structure refinement was also covered. The structure of the workshop was very interactive with lectures followed by (or along with) hands-on sessions.
12. Benefit/Key outcomes of the Program /activity/ event	Participants benefitted from this workshop and were satisfied with the workshop for conducting highly informative technical sessions, and improving their soft skills by using crystallographic softwares with X-ray diffraction data.
13. Enclosures with report	Detailed report, Workshop brochure, Registration details, Photos of the workshop sessions are enclosed.



Dr. Hari K. Kadam
Coordinator
Goa University Crystallography Workshop - 2024



Prof. V. M. S. Verenkar
Dean, School of Chemical Sciences
Goa University





GOA UNIVERSITY

SCHOOL OF CHEMICAL SCIENCES

Goa University Crystallography Workshop – 2024

23rd & 24th October 2024

Detailed Report

School of Chemical Sciences (SCS), Goa University, organized a Goa University Crystallography Workshop - 2024 (GUCW-II); a DST-PURSE funded Two-days National level workshop on Materials Characterization using Powder X-ray Diffraction on 23rd & 24th October 2024 at Chemistry Auditorium, School of Chemical Sciences, Goa University.

The objective of this workshop was to provide in-depth knowledge and hands-on training on powder X-ray diffraction techniques.

Honourable Vice-Chancellor of Goa University Prof. Harilal B. Menon graced the inaugural session as the chief Guest. Other dignitaries on the dais were Dean, SCS Prof. Vidhyadatta M. S. Verenkar, Goa University DST-PURSE Coordinator Prof. Rajendra Gad and Workshop Coordinator Dr Hari Kadam. Dean, SCS welcomed all for the workshop and briefed the participants about School. All the dignitaries inaugurated the workshop with lighting of lamp. Hon. VC addressed the gathering and appreciated the nation-wide response for the workshop. He stressed upon the study of crystal structure in Mineralogy, Space exploration, Energy storage materials, pharmaceuticals, constructions, superconductors, nano-composites, forensic sciences, Archeology, Polymers, etc. Vote of thanks for the inaugural session was delivered by Dr. Hari Kadam.

Resource Person for the workshop were:

- Dr. Tapas Kumar Mandal; Associate Professor, IIT Roorkee
- Dr. Diptikanta Swain; Scientific Officer, ICT-IOC Bhubaneswar
- Dr. Digamber Porob; Associate Professor, Goa University
- Dr. Elaine T. Dias; Assistant Professor, Goa University

Technical sessions were Chaired by Workshop Coordinator: Dr Hari Kadam, Vice Dean (Academic) Prof. Sunder Dhuri, Vice Dean (Research) Dr. Bidhan Shinkre and Program Director (Biochemistry) Dr. Prachi Torney.

Common crystallographic softwares like WinPLOTR and Fullprof were used for hands-on training in indexing, whole powder pattern fitting, and Rietveld refinement. Multi-phase Rietveld refinement and magnetic structure refinement was also covered. The structure of the workshop was very interactive with lectures followed by (or along with) hands-on sessions.

All Participants were advised to carry their own laptop. Participants worked on preloaded software on their laptop. Download link and installation instructions were shared by organizing team to the registered participants. Hands-on sessions were conducted to learn the concepts by solving problems of different complexity levels (simple to advanced).

Technical sessions were conducted with following titles:

- Introduction to Powder X-ray Diffraction and Data Collection Strategies
- Indexing of Powder Diffraction Pattern - Hands on Training Using WinPLOTR
- Whole Powder Diffraction Pattern fitting – Hands on Training Using WinPLOTR - Fullprof Suite
- Introduction to Rietveld Refinement - Hands on Training Using WinPLOTR - Fullprof Suite
- Magnetic Structure refinement and Multi Phase Rietveld Refinement – Hands on Training
- Structural elucidation of powder samples by combining X-Ray, Electron diffraction and TEM Techniques
- Use of Powder Diffraction with other techniques

This workshop was mainly intended for Post-Graduate and Ph.D students and faculties in chemistry, physics and related fields of material sciences who have basic knowledge of crystallography. Participation for this workshop was invited from interested students and faculties of the Universities, institutes, colleges, from across the country.

172 Students and 35 Faculty Participants from following institutions attended the workshop:

Cochin University of Science and Technology (CUSAT), Kochi
CSIR- Indian Institute of Chemical Technology (IICT), Hyderabad
CSIR- National Chemical Laboratory (NCL), Pune
Dr Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajnagar
IISER Bhopal
IISER Mohali, Punjab
Netaji Subhas University of Technology, New Delhi
Manipal Institute of Technology, Manipal
Mangalatayan University, Jabalpur, Madhya Pradesh
Central University of Himachal Pradesh, Kangra, Himachal Pradesh
BITS Pilani, Goa
Government College of Arts, Science and Commerce, Quepem, Goa
P.E.S's R.S.N. College of Arts and Science, Ponda, Goa
P.E.S's Rajaram and Tarabai Bandekar College of Pharmacy, Ponda, Goa
Parvatibai Chowgule College of Arts and Science, Margao, Goa
St. Xavier's College, Mapusa, Goa
School of Biological Sciences and Biotechnology, Goa University
School of Physical & Applied Sciences, Goa University
School of Chemical Sciences, Goa University

Participants were also taken to visit Goa University Research Park Unit (GURU) and Prof. Sandeep Garg showed and explained the various instrumental and infrastructural facilities

developed by Goa University to support innovation and start-ups. Participants were also shown the infrastructural and instrumental facilities available in SCS.

Participants benefitted from this workshop and were satisfied with the workshop for conducting highly informative technical sessions, and improving their soft skills by using crystallographic softwares with x-ray diffraction data.

Honourable Registrar of Goa University Prof. Vishnu S. Nadkarni was the Chief Guest for Valedictory session. Other dignitaries on the Dais were Dean, SCS Prof. V. M. S. Verenkar, Goa University DST-PURSE Coordinator Prof. Rajendra Gad, Workshop Coordinator Dr Hari Kadam, Workshop Co-Coordinators Dr. Prajesh Volvoikar and Dr. Kiran Dhavskar. Dignitaries were welcomed by Dr. Prajesh Volvoikar. Chief Guest addressed the gathering and appreciated the participants from across the country for participating in this workshop. Participants were invited for sharing their experience and feedback on workshop. Participants from other institutes were handed over participation certificates by the Chief Guest. Vote of Thanks was delivered by Dr Kiran Dhavskar.

Workshop brochure, Registration sheets, Photos of the workshop sessions are enclosed.



Dr. Hari K. Kadam
Coordinator
Goa University Crystallography Workshop - 2024



Prof. V. M. S. Verenkar
Dean, School of Chemical Sciences
Goa University





विज्ञान एवं प्रौद्योगिकी विभाग
DEPARTMENT OF
SCIENCE & TECHNOLOGY



GOA UNIVERSITY

SCHOOL OF CHEMICAL SCIENCES (SCS)

ORGANISES

GOA UNIVERSITY CRYSTALLOGRAPHY WORKSHOP - 2024 (GUCW-II)

**TWO-DAYS NATIONAL LEVEL
WORKSHOP ON
MATERIALS CHARACTERIZATION
USING POWDER X-RAY DIFFRACTION**

Funded by:

DST-PURSE

Dates: 23rd & 24th OCTOBER 2024

**Venue: Chemistry Auditorium,
School of Chemical Sciences (SCS),
Block E, Goa University,
Taleigao Plateau, Goa 403206 India**

ABOUT GOA UNIVERSITY

Goa University was established under the Goa University Act of 1984 (Act No. 7 of 1984) and commenced operations on 1st June 1985. The University took over the enhanced role of the Centre of Post-Graduate Instruction and Research (CPIR) which was set after the liberation of Goa by India in December 1961, by the University of Bombay (now Mumbai), in June 1962. Since 1985 Goa University has offered graduate and post-graduate studies and research programs.

SCHOOL OF CHEMICAL SCIENCES (SCS)

The establishment of the School of Chemical Sciences took place by transforming one of the existing and oldest (established in 1965 as a part of Centre for Post-Graduate Instruction and Research of the then Bombay University) department (of Chemistry) into a School. The School is currently located in the faculty block E since April 2013, with modern infrastructure, conducive for quality education and research in Chemistry. The School (formerly Department of Chemistry) earlier had Organic, Inorganic, Physical and Analytical Chemistry as distinct streams and since AY 2019-20, the Biochemistry has been added as its fifth stream. The research at this School has been recognized by the award of projects to the individual faculty members and also receiving handsome grants from the University Grants Commission (UGC) and the Department of Science & Technology (DST), Govt. of India in their prestigious programs like UGC-SAP and DST-FIST. The School of Chemical Sciences has various modern sophisticated instruments required for state-of-the-art research.

PATRON

Prof. Harilal B. Menon

Hon. Vice-Chancellor, Goa University

Workshop Coordinator

Dr. Hari K. Kadam

Co-Coordinators

Dr Prajesh S. Volvoikar

Dr Kiran T. Dhavskar

Organising Committee

Prof. Vidhyadatta M. S. Verenkar
(Dean, SCS)

Prof. Rajendra S. Gad
(Goa University DST-PURSE Coordinator)

Prof. Kaustubh R. S. Priolkar

Prof. Sunder N. Dhuri

Dr. Digamber G. Porob

Dr. Rupesh E. Patre

Dr Bidhan A. Shinkre

Dr. Sudhir Cherukulappurath

Dr. Venkatesha Hathwar

Contact Details

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Dr Prajesh S. Volvoikar ([7030965977](tel:7030965977))

Dr Kiran T. Dhavskar ([7030699157](tel:7030699157))

gucw@unigoa.ac.in

INVITED SPEAKERS



Dr Tapas Kumar Mandal
(IIT Roorkee)



Dr Diptikanta Swain
(ICT-IOC Bhubaneswar)



Dr. Digamber Porob
(Goa University)



Dr. Elaine T. Dias
(Goa University)

ABOUT THE WORKSHOP

The primary objective of this workshop is to provide in-depth knowledge and hands-on training on powder X-ray diffraction techniques. Common crystallographic softwares like WinPLOTR and Fullprof will be used for hands-on training in indexing, whole powder pattern fitting, and Rietveld refinement. Multi phase Rietveld refinement and magnetic structure refinement will also be covered.

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).

REGISTRATION

Online Registration is compulsory.

Registration Fees:

Rs. 500/- for PG & PhD students of affiliated colleges of Goa University.

Rs. 1,000/- for the teachers of affiliated colleges of Goa University.

Rs. 1,000/- for PG & PhD students of all other institutes not affiliated to Goa University.

Rs. 2,000/- for the teachers of all other institutes not affiliated to Goa University.

Rs. 3,000/- for participants from Industry.

Rs. NIL for students and teachers of Goa University

Rs. 5,000/- for spot registration in all above categories after last date of registration.

Payment should be done only after receiving acceptance email for participation.

Last Date for Registration is 07/10/2024

[CLICK HERE FOR REGISTRATION FORM](#)

The number of participants is limited to 100

IMPORTANT INFORMATION TO PARTICIPANTS

This workshop is mainly intended for Post-Graduate and Ph.D students in chemistry, physics and related fields of material sciences who have basic knowledge of crystallography.

The workshop is also open to interested faculty members of the University, institutes, and colleges, as well as from the industry.

Participation is confirmed only after receiving confirmation email from the workshop organizing team.

All Participants should carry their own laptop with atleast 30 min battery backup. Participants will work on preloaded software on their laptop. Download and installation instructions will be communicated after registration.

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.

Day 1: Wednesday, 23rd OCTOBER 2024

9:30 - 10:00am	Registration
10:00 - 10:30am	Inaugural session
10:30 - 11:00am	TEA BREAK
11:00 - 1:00pm	Technical Session - i (Dr. Digamber G. Porob) Introduction to Powder X-ray Diffraction and Data Collection Strategies
1:00 - 2:00pm	LUNCH
2:00 - 3:30pm	Technical Session - ii (Dr. Tapas K. Mandal) Indexing of Powder Diffraction Pattern - Hands on Training Using WinPLOTR
3:30 - 4:00pm	TEA BREAK
4:00 - 5:30pm	Technical Session - iii (Dr Diptikanta Swain) Whole Powder Diffraction Pattern fitting – Hands on Training Using WinPLOTR - Fullprof Suite

Day 2: Thursday, 24th OCTOBER 2024

9:30 – 11:00am	Technical Session - iv (Dr Diptikanta Swain) Introduction to Rietveld Refinement - Hands on Training Using WinPLOTR - Fullprof Suite
11:00 – 11:30am	TEA BREAK
11:30 – 1:00pm	Technical Session - v (Dr Elaine T. Dias) Magnetic Structure refinement and Multi Phase Rietveld Refinement – Hands on Training
1:00 - 2:00pm	LUNCH
2:00 - 3:30pm	Technical Session - vi (Dr. Tapas K. Mandal) Structural elucidation of powder samples by combining X-Ray, Electron diffraction and TEM Techniques
3:30 - 4:00pm	TEA BREAK
4:00 - 5:00pm	Technical Session - vii (Dr Diptikanta Swain) Use of Powder Diffraction with other techniques
5:00 - 5:30pm	Valedictory Q&A, Concluding remarks and Feedback from participants

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SCHOOL OF CHEMICAL SCIENCES**

GOA UNIVERSITY CRYSTALLOGRAPHY WORKSHOP - 2024 (GUCW-II)

DST-PURSE funded

Two-days National level workshop on Materials Characterization using Powder X-ray Diffraction

on 23rd & 24th OCTOBER 2024 at Chemistry Auditorium, School of Chemical Sciences, Goa University

FACULTY PARTICIPANTS (INSTITUTES NOT AFFILIATED TO GOA UNIVERSITY)

Sr No	Full Name	Email ID	Institute/Organization	Registration fees Rs.	Fees paid participation confirmed	Sign
1	Dr Saurav Bhattacharya	sauravb@goa.bits-pilani.ac.in	BITS Pilani, Goa	2000	DUN1696773 14/09/2024	<i>S. Bhattacharya</i>
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4	Dr. K. Krishna Murthy Goud	krishnamurthy.k@uceou.edu	University College of Engineering, Osmania University, Hyderabad	2000	DUN2165644 26/09/2024	
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8	Dr. Bidyutjyoti Dutta	bidyutjyoti.dutta436@gmail.com	IISER Mohali, Punjab	2000	DUN2425971 03/10/2024	<i>Bidyutjyoti Dutta</i>

↓
*Mangalatayan University,
Jabalpur*

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STUDENTS PARTICIPANTS (INSTITUTES NOT AFFILIATED TO GOA UNIVERSITY)

Sr No	Full Name	Email ID	Institute/Organization	Registration fees Rs.	Fees paid participation confirmed	Sign
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13	Lohith Kotte	kottelohith@gmail.com	CSIR- Indian Institute of Chemical Technology (IICT), Hyderabad	1000	DUN1873474 19/09/2024	<i>Lohith</i>
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STUDENTS PARTICIPANTS (INSTITUTES NOT AFFILIATED TO GOA UNIVERSITY)

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STUDENTS PARTICIPANTS (INSTITUTES NOT AFFILIATED TO GOA UNIVERSITY)

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FACULTY PARTICIPANTS (AFFILIATED INSTITUTES)

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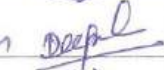

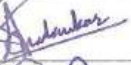


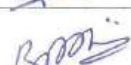
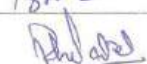
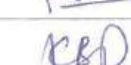
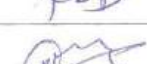


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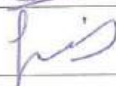




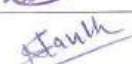
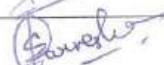
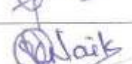







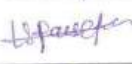
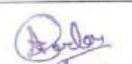

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


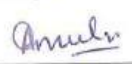
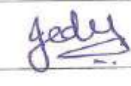



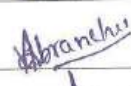

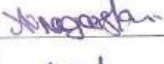




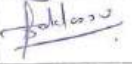
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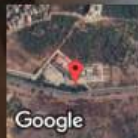
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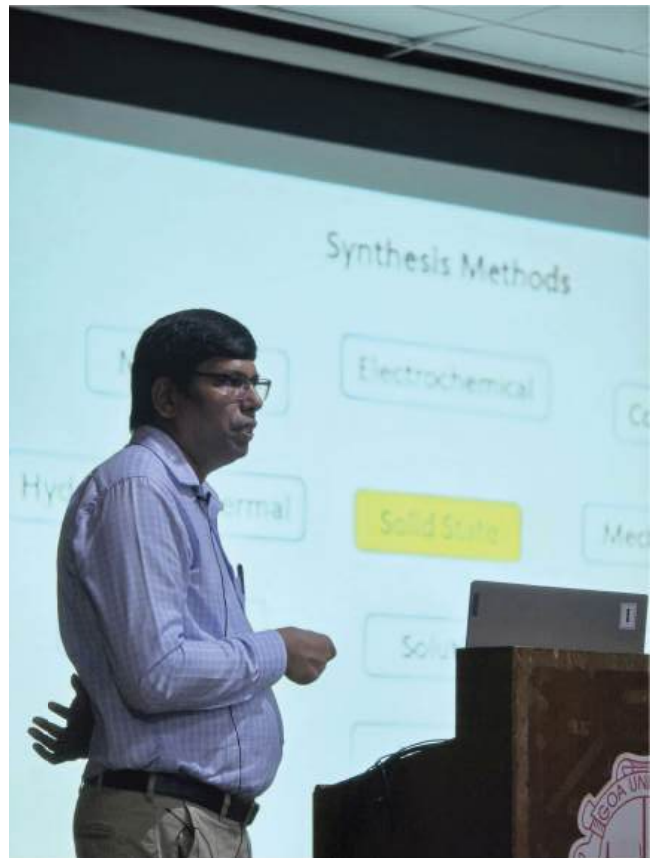
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