

1<sup>ST</sup> ONLINE HANDS-ON-TRAINING ON  
**RIETVELD REFINEMENT OF X-RAY DIFFRACTION (RRD)**  
(USING FULLPROF SOFTWARE PACKAGE)

Centre for Advanced Computational Research, New Delhi, India

(Registered under Ministry of SME, Government of India for Research and Experimental Development on Natural Sciences and Engineering)  
(ISO 9001:2015 Certification for Hands-on-Training on Computational Science including DFT calculation of Materials, Molecular Docking and Dynamics)  
Website: <https://cacrdelhi.com>, Email: [admin@trainingcacrdelhi.com](mailto:admin@trainingcacrdelhi.com)

|Space Group Determination| |Indexing (h k l)|, |Profile Fitting| |Crystallite Size-Strain Analysis| |Lattice Parameter Calculation| |Williamson-Hall Plot| |Phase Identification|  
|Theoretical X-ray Diffraction Pattern|

**[Online + Recordings]** Date: 8<sup>th</sup> April – 14<sup>th</sup> April 2025

Timing: **Morning Batch:** 9:00 AM – 10:00 AM IST or **Evening Batch:** 9:00 PM – 10:00 PM IST

**[Online Live Sessions along with Complete Recordings]**

## 1. About Us

Centre for Advanced Computational Research, New Delhi, India, established in April 2021, is an International Research unit with research focus in Materials Sciences, Analytical chemistry, Organic & Inorganic chemicals synthesis, Pharmaceuticals and Bioinformatics. The R&D activities primarily involve the in-depth spectroscopic studies of Novel material via modern computational chemistry/physics approaches toward their applications in organic light-emitting diodes (OLEDs), Photovoltaics, catalysis, Optoelectronic devices, polymer design, energy-based materials, non-linear optical activity, energy transfer mechanisms, and Bioinformatics. The organization is headed by Dr. Nikhil Aggarwal along with 15 External Faculty Members and 18 project students from the premier research institutions of India and abroad including IISc Bangalore, IITs, NITs, CSIR Labs, etc. We are also actively engaged in promoting Computational Sciences via online Workshops/Hands-on-Training. We are proud to say that we are the first to introduce Hands-on-Training (Online and Onsite) on Quantum Chemical calculation via Density Functional Theory Approach. In a short span of 4 years, we have trained **8000+** Graduate students, Research Scholars, Professors &

Industry Experts from 35 countries including the India, US, UK, Saudi Arabia, Mexico, Brazil, Malaysia, Kuwait, Germany, Peru, South Korea, Finland, Turkey, Iraq, Australia, Philippines, Spain, Jordan, Chile, Taiwan, South Africa, Pakistan, Nepal, Bangladesh, Nigeria, Morocco, Egypt, Sri Lanka and Algeria, Singapore, Columbia, Sweden, Botswana, Belgium, Canada and rated 4.78/5.00 by 700+ International and National participants of our previous workshops. Centre previously had 5 invited lectures:

1. **Dr. Snehasis Daschakraborty**, Asst. Prof. (IIT Patna):[\[https://www.youtube.com/watch?v=CaZl0iFJU-I\]](https://www.youtube.com/watch?v=CaZl0iFJU-I)
2. **Prof. T. P. Radhakrishnan**, Prof. (Hyderabad University):[\[https://www.youtube.com/watch?v=5IWNLsntgSU\]](https://www.youtube.com/watch?v=5IWNLsntgSU)
3. **Dr. V. Ramanathan**, Asst. Prof. (IIT BHU):[\[https://www.youtube.com/watch?v=erKb3y71VN8\]](https://www.youtube.com/watch?v=erKb3y71VN8)
4. **Prof. Kalidas Sen**, Prof. (Emeritus) (Hyderabad University):[\[https://www.youtube.com/watch?v=jkz\\_Hb99vEg\]](https://www.youtube.com/watch?v=jkz_Hb99vEg)
5. **Dr. Ranganathan Subramanian**, Associate Professor (IIT Patna).



**Prof. T. P. Radhakrishnan**  
 Professor [University of Hyderabad]  
 H-Index = 38, Citations = 5046  
 FNASc, FASc, FNA, Ph. D., Princeton University  
 Postdoctoral Research, University of Texas at El Paso



**DR. SNEHASIS DASCHAKRABORTY**  
 Assistant Professor [IIT Patna]  
 H-Index = 15, Citations = 702  
 Postdoctoral Research, University of Colorado



**DR. RANGANATHAN SUBRAMANIAN**  
 Associate Professor, IIT Patna  
 H-Index = 7, Citations = 550  
 Ph.D, Wesleyan University



**PROF. KALIDAS SEN**  
 Professor (Emeritus), Hyderabad University  
 H-Index = 42, Citations = 6024  
 F.A.Sc., F.N.A.



**DR. V. RAMANATHAN**  
 Assistant Professor [IIT BHU]  
 H-Index = 11, Citations = 529  
 Postdoctoral Research, University of Stuttgart, Germany

## 2. About FDP/Workshop (Hands-on-Training) Program:

We are glad to announce **7-Days Online FDP/Workshop (Hands-on-Training) program on Rietveld Refinement of X-Ray Diffraction Data (RRD) (Hands-on-Training using Free Licence Software Tool: FullProf Software package)**. There has been a renaissance in powder diffraction in recent years because Rietveld refinement allows determinations of positional and thermal parameters from powder data, even when the diffraction peaks are not well separated in the recorded pattern. In a polycrystalline sample, information may be lost as a result of the random orientation of the crystallites. Rietveld developed a refinement method that uses the profile intensities of the composite peaks instead of the integrated quantities. This is a pattern-fitting method of structure refinement and allows extraction of the maximum amount of information contained in the powder pattern.

- ✓ The Hands-on-training Program is planned for **Faculty (FDP Completion Certificate)** and **Post-docs, Research Scholars, post-graduate students (Certification of Training completion)**.
- ✓ Training Session is designed as per the guidelines defined by the **UGC** and can be used for **Research Articles publication**.
- ✓ The **required free software's for training will be provided**. We understand the Academic schedules of participants so **complete lecture recordings** will be given to all participants.

## 3. Please visit below webpage and submit your Registration Form and Fees

<https://www.cacrdelhi.com/event-details/7-days-online-fdp-workshop-hands-on-training-on-rietveld-refinement-of-x-ray-diffraction-data-using-fullprof-package-2>

or

<https://www.cacrdelhi.com/rrd-refinement>

#### 4. Day wise Schedule

##### 8<sup>th</sup> April 2025: Day 1 Session 1

- Rietveld Refinement of X-ray Diffraction Data Using FullProf Package
- Rietveld Refinement of X-ray Diffraction Data of **Doped Samples** Using FullProf Package

##### 9<sup>th</sup> April 2025 Day 2 Session 2

- Rietveld Refinement of X-ray Diffraction Data of **NBT** Using FullProf Package
- **Space Group Determination & Indexing** from XRD Data

##### 10<sup>th</sup> April 2025 Day 3 Session 3

- **Instrumental Resolution File (IRF)** for Rietveld Refinement Using FullProf Package
- Rietveld Refinement Study of Some **Perovskite Type Solid Solutions**: Theory and Application

##### 11<sup>th</sup> April 2025 Day 4 Session 4

- **Profile Fitting** and **Crystallite Size-Strain Analysis**

##### 12<sup>th</sup> April 2025 Day 5 Session 5

- **Lattice Parameter Calculation** and **Indexing (h k l)**

##### 13<sup>th</sup> April 2025 Day 6 Session 6

- **Williamson-Hall Plot** from XRD Rietveld Analysis: Crystallite Size and Strain
- **Phase Identification** Using Rietveld Fit

##### 14<sup>th</sup> April 2025 Day 7 Session 7

- Simulate a **Theoretical X-ray Diffraction Pattern from CIF File** for Phase Identification

#### 5. Registration Category and Fees

Registration Type	International	National
Faculty or Scientific officer	USD 65	Rs. 2,500
Post-doctorate's Participants	USD 55	Rs. 2,000
Research Scholars and other Participants	USD 45	Rs. 1,500
Undergraduate or Postgraduate	USD 35	Rs. 1,000

#### 6. Salient Features

- ✓ **Eligibility:** Candidate must have knowledge of undergraduate level science.
- ✓ Hands-on-Training sessions will be taken via online mode: ZOOM, Lecture Mode: English
- ✓ e-certificates will be provided to all registered participants (**minimum 2/7 attendance**)
- ✓ Training will be provided on Windows Operating system
- ✓ Programming and coding knowledge is **not required** for above Hands-on-Training.

**Contact at:**

[admin@trainingcaacrdelhi.com](mailto:admin@trainingcaacrdelhi.com), [nikhilaggarwal@alumni.iitm.ac.in](mailto:nikhilaggarwal@alumni.iitm.ac.in)

+91 9790969349 via call or WhatsApp message for any query.

**Certificate (Copy) to be issued.**

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**Certificate of FDP Completion**

This is to certify that

**Utkarsh Verma, Professor, India**

has actively participated in the 1<sup>st</sup> Faculty Development Program (FDP) on Rietveld Refinement of X-Ray Diffraction (RRD) organized by the Centre for Advanced Computational Research, Delhi from 8<sup>th</sup> – 14<sup>th</sup> April 2025 via Online Mode. FDP had 7 Interactive Sessions by DR. NIKHIL AGGARWAL on Rietveld Refinement of X-Ray Diffraction data using FullProf Software Package.

**Dr. Nikhil Aggarwal**  
Head of the Department & Convener



ISO Accreditation Body **United Accrediting Services Limited, United Kingdom**  
Certificate No.: 2025/RRD/F/1/1

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