



**Dr. Sanjit Konar** is an Associate Professor of Chemistry at IISER Bhopal. His research interests are Nanomagnets, MOF materials, polyoxometallates for catalysis, and nanoscopic molecular clusters and cages.



**Dr. Shaikh M. Mobin** is an Associate Professor at IIT Indore. His group focuses on single-source molecular precursors (SSMP) for the synthesis of functional nanomaterials.



**Prof. Sujit K. Ghosh** is a Professor of Chemistry at IISER Pune. His research efforts are focused in the areas of metal-organic frameworks, porous organic frameworks, and metal-organic polyhedra.



**Prof. Jitendra K. Bera** is a Professor of Chemistry at IIT Kanpur. His group focuses their efforts in organometallic catalysis for small-molecule activation. His group prepares various polynuclear metal constructs and study their catalytic activity.



**Prof. Arijit Mukherjee** is an Assistant Professor at BITS Pilani, Hyderabad Campus. His research interests are in the crystal engineering of organic solids, polymorphs, APIs, the design of functional materials among others.



**Dr. Prathapa Siriya Jagannatha** is a Product Manager and Application Scientist SC-XRD Bruker India Scientific Pvt. Ltd. His topic of interests is structure solution and data refinement.

## Registration & Contact Details

- Interested participants must register and only selected candidates would be invited for the workshop.
- For selected candidates Registration fees, local travel, Boarding and lodging will be covered by DST.

Interested participants should register using the following link:

<https://forms.gle/1DApgKYueBmgqAbL8>

**Registration Deadline: Aug. 12, 2022.**

Shortlisted candidates will be intimated by email, latest by Aug. 16, 2022.

### Eligibility criteria:

- Minimum qualification: Post-Graduate (Science) or B.Tech. (Technology).
- Professors/Scientists/Post-Doctoral Fellows/Ph.D. Fellows/Industry persons who are actively involved in R&D.
- Not more than 2 participants from an institute.

### For more information:

**Coordinator: Dr. Manju S. L.**

**Access:** <https://vit.ac.in/school-advanced-sciences-sas/one-week-workshop-x-ray-crystallography-and-determination-molecular>

&

<https://events.iitgn.ac.in/stuti/>

**Mail:** [dststuti.vit@vit.ac.in](mailto:dststuti.vit@vit.ac.in)

**Address:** Department of Chemistry,  
School of Advanced Sciences,  
Vellore Institute of Technology,  
Vellore, 632014, India.

## Acknowledgements



सत्यमेव जयते

Department of Science & Technology  
Govt. of India



Department of Science & Technology  
(DST) Funded  
**Training Workshop Under STUTI**  
(Synergistic Training Program Utilizing  
the Scientific and Technological  
Infrastructure)

**One Week Workshop on  
X-Ray Crystallography and  
Determination of Molecular  
Structure**

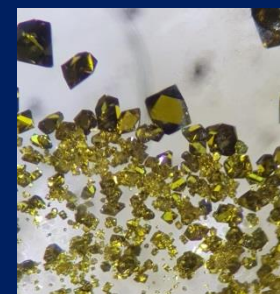
**Aug. 22 – 28, 2022.**



**VIT<sup>®</sup>**

**Vellore Institute of Technology**  
(Deemed to be University under section 3 of UGC Act, 1956)

Department of Chemistry,  
School of Advanced Sciences,  
Vellore Institute of Technology, Vellore.



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**Dr. Rajagopal D**

*HoD, Chemistry*

### Coordinator

**Dr. Manju S L**

### Organizing Team

**Dr. Palanisami N**

**Dr. K. R. Ethiraj**

**Dr. Asharani I.V**

**Dr. Arup Sinha**

**Dr. Cheralathan K.K**

**Dr. Tamas Kumar Panda**

**Dr. Manish Kumar Mishra**

**Dr. Logesh Mathivathanan**

**Ms. Sherin Anto**

**Dr. Rajasekhara Reddy S**

**Dr. Mohana Roopan S**

Contact details: [dststuti.vit@vit.ac.in](mailto:dststuti.vit@vit.ac.in)

**About VIT:** VIT was founded in 1984 as Vellore Engineering College by the Hon. Chancellor Dr. G. Viswanathan with the aim of providing quality higher education on par with international standards. It persistently seeks and adopts innovative methods to improve the quality of higher education on a consistent basis. National Assessment and Accreditation Council (NAAC) has re-accredited (IV Cycle) with a CGPA of 3.66 on a seven point scale at 'A++' Grade. VIT has been ranked 10<sup>th</sup> in Research, 12<sup>th</sup> in Engineering Category, 9<sup>th</sup> in University Category and 18<sup>th</sup> in Overall Category by the MHRD-NIRF Ranking 2022.

**School of Advanced Sciences (SAS)** is pledged to internationally acclaimed research and inventive instruction with a priority on disciplinary rigor and establish academic achievement. It comprises three academic departments spanning Chemistry, Physics & Mathematics. In QS world ranking by subject Chemistry Top 401-450, Mathematics Top-451-500 and THE ranking for Physical Sciences 601-800.

### Programs Offered at VIT

The School offers M. Sc. Physics, RSC accredited M.Sc. Chemistry (Organic/Inorganic/Analytical/Pharma) M. Sc. (Data Science), M. Sc. Integrated Five Year Programs (Computational Statistics and Data Analytics, Chemistry, Physics and Mathematics) and Ph. D. programs.

### Overview of STUTI and Objectives of the Workshop

DST welcomes all the participants for the workshop on Single Crystal X-Ray crystallography organised under STUTI. The STUTI program envisions hands-on-training and sensitization of the state-of-the-art equipment as well as towards sharing while ensuring transparent access to S&T facilities. Department of Science and Technology has identified IIT Gandhi Nagar (IITGN) as the Project Management Unit (PMU) and VIT as the coordinator for this workshop.

VIT Vellore is home to state-of-the-art instrumentation for SCXRD and the workshop will explore the theory and practice involved in various stages of molecular structure determination. Expert talks will provide our vision for the use of crystallography beyond simple structure determinations. We will highlight unusual problems faced in structure determination and provide solutions through expert lectures and hands-on training.

### Contents of the workshop

#### Day 1 - Aug. 22, 2022

**Inaugural session-Expert Talk** by Dr. Sanjit Konar

**Hands-on Session:** Introduction to single crystals and crystallization techniques – Dr. Arup Sinha and Dr. Logesh Mathivathanan

#### Day 2 - Aug. 23, 2022

**Expert Talk** by Dr. Shaikh M. Mobin and Dr. Arup Sinha

**Hands on Session:** Lab Visit, crystallization techniques -Dr. Asha Rani IV

#### Day 3 - Aug. 24, 2022

**Expert Talk** by Dr. Manish Kumar Mishra and Dr. Tamas Kumar Panda

**Hands-on:** Crystal screening and data collection - Dr. Palanisami N

#### Day 4 - Aug. 25, 2022

**Expert Talk** by Prof. Sujit Ghosh and Dr. Logesh Mathivathanan

**Hand on:** Crystal selection, mounting & centering- Ms. Sherin

#### Day 5 - Aug. 26, 2022

**Expert Talk** by Prof. Jitendra K. Bera and Dr. Prathapa Jagannadha

**Hands on:** Strategy optimizer & setting up a measurement Data reduction, scaling & structure solution - Dr. Manju S L

#### Day 6 - Aug. 27, 2022

**Expert Talk** by Dr. Arijit Mukherjee

**Hands-on:** Structure solution and refinement - Ms. Sherin Anto

#### Day 7 - Aug. 28, 2022

**Interactive and Problem-solving session followed by closing remarks.**

### SCHEDULE

#### Day 1, 22/8/2022

08:30 Registration  
09:00 Inaugural Session  
10:45 Tea Break  
11:00 Expert Talk 1  
12:30 Lunch  
14:00 Session II (Hands on)  
16:30 Tea Break  
16:45 Campus Visit

#### Day 2, 23/8/2022

09:00 Expert Talk 2  
11:00 Break  
11:30 Expert Talk 3  
12:30 Lunch  
14:00 Session II (Hands on)  
16:30 Tea Break  
16:00 Lab visit

#### Day 3, 24/8/2022

09:00 Expert Talk 4  
11:00 Tea Break  
11:30 Expert Talk 5  
12:30 Lunch  
14:00 Session IIA  
15:30 Tea Break  
16:00 Session IIB  
17:00 Discussion

#### Day 4, 25/8/2022

09:00 Expert Talk 6  
11:00 Tea Break  
11:30 Expert Talk 7  
12:30 Lunch  
14:00 Session IIA  
15:30 Tea Break  
16:00 Session IIB  
17:00 Discussion

#### Day 5, 26/8/2022

09:00 Expert Talk 8  
11:00 Tea Break  
11:30 Expert Talk 9  
12:30 Lunch  
14:00 Session IIA  
15:30 Tea Break  
16:00 Session IIB  
17:00 Discussion

#### Day 6, 27/8/2022

09:00 Expert Talk 10  
11:00 Tea Break  
11:30 Expert Talk 11  
12:30 Lunch  
14:00 Session IIA  
15:30 Tea Break  
16:00 Session IIB  
17:00 Discussion

#### Day 7, 28/8/2022

09:00 Interactive session  
11:15 Tea Break  
11.30 Closing remarks

**Networking  
Dinner on Day 5**